USERS' MANUAL FOR SAMM2, SHARC-4 and MODTRAN4 MERGED

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14. ABSTRACT
The SAMM2 (SHARC and MODTRAN Merged Code version 2) combines the capabilities of the Strategic High-Altitude Radiance Code, SHARC-4, and MODerate resolution TRANsmittance code, MODTRAN4. The code calculates atmospheric Infrared radiance and transmission over a 1 - 40 μm spectral region for arbitrary lines of sight (LOS) from the ground to 300 km altitude using an approximate line-by-line radiative transport (RT) algorithm capable of a fine spectral resolution of 0.001 cm^{-1}. It models molecular emissions due to non-local thermodynamic equilibrium (NLTE) conditions at high altitudes (>50 km) and local thermodynamic equilibrium (LTE) conditions at lower altitudes (<50 km). This second version of SAMM has been upgraded to include single and multiple scattering effects by clouds and/or aerosols, which can be specified by the user via an interactive input menu. SAMM2 predicts atmospheric structure due to stochastic processes described by a temperature and density fluctuation model. The radiance statistics are non-stationary and are dependent on sensor bandpass, location and field of view (FOV). The code includes the ability to perform multiple LOS calculations during a single execution. Auxiliary atmospheric profile generator and slit function programs enhance the capabilities of the code. As in previous versions of the code, auroral regions can be embedded in quiescent atmospheres, the atmospheric terminator can be treated, and industry-standard kinetics and radiation transport modules have been employed. This manual outlines the scientific basis of the code, details steps for code installation and use as supplied, and indicates how the user may modify the supplied input files if desired.

15. SUBJECT TERMS
Infrared radiation, Atmospheric radiance, Atmospheric structure, LTE/NLTE, Multiple scattering, Line-by-Line

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1. INTRODUCTION

This manual describes SAMM2, the second major release of the SHARC and MODTRAN MERGED Code, which is a combination of SHARC-4 and MODTRAN4. It briefly discusses the underlying phenomenology and aids the user in running SAMM2 by providing code implementation instructions and illustrative interactive sessions. As with the atmospheric codes previous releases [Sharma *et al.*, 1989; Sharma *et al.*, 1991; Sharma *et al.*, 1996a; Sharma *et al.*, 1996b; Gruninger *et al.*, 1996], SAMM2 predicts infrared (IR) atmospheric radiation and transmittance in the 2 - 40 μm spectral region and includes important bands of NO, CO, H_2O, O_3, OH, CO_2, CH_4, HNO_3, N_2O, NO_2, SO_2, NH_3, and NO^+. For OH, the wavelength range is extended to 1 μm to include the spectral radiance from the OH($\Delta v=2$) transitions near 1.4 μm. The primary upgrade included in SHARC-4 was the addition of a model for atmospheric background radiance structures and the capability to perform calculations for a series of lines-of-sight during a single execution of the code. The radiance structures result from fluctuations in the density of atmospheric species, individual molecular state populations, and kinetic temperatures and pressures along the sensor line-of-sight (LOS). SHARC-4 predicts a two dimensional radiance spatial covariance function from the underlying 3D atmospheric structures. The radiance statistics are non-stationary and are dependent on sensor bandpass, location and field of view (FOV). The new SAMM2 modeling capabilities dealing with radiance structures are discussed in detail in section 2.4.

SAMM2 was developed as a modular code so that models and model parameters can be easily modified or upgraded as additional data and/or better models become available. The framework is thus different from that of SHARC-4 and MODTRAN4, comprising a completely new architecture. SAMM2 is thus a completely new code and not merely a revision of SAMM1. The present modules include input, ambient chemistry, time-dependent auroral chemistry, radiative transport, geometry (including refractive geometry), radiance structure, and output. The input module is interactive, menu-driven, and checks all input parameters for validity before continuing with the calculation. The SAMM2 radiative transport includes single and multiple scattering by clouds and/or aerosols, as well as ground reflectance, which can be specified via the menu driven input module. SAMM2 therefore covers the entire altitude range from ground to space and models both the LTE (Local Thermodynamic Equilibrium) and NLTE (Non Local Thermodynamic Equilibrium) regimes. An

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ongoing upgrade, to appear in a future release, is the development of a two-temperature rotational distribution for OH and NO, motivated by results from the CIRRIS 1A experiment [Smith *et al.*, 1992; Joseph *et al.*, 1989; Sharma *et al.*, 1998].

The following is the calculational sequence for a SAMM2 calculation which utilizes the new radiance structure and multiple scattering features. First the input module prepares the inputs required by the rest of the code. These inputs include a description of the atmospheric temperature statistics and the range of the geometry parameters encompassing the physical extent of the observed scene, as well as specification of aerosols and/or cloud models, and ground reflectance. The next step is calculation of the mean excited-state populations and fluctuations of the populations about the mean due to local density and temperature fluctuations. This is accomplished in the chemistry ambient module. The ambient population module iterates between a generalized chemical kinetics module [Kee *et al.*, 1980] that calculates excited-state populations due to solar and earthshine excitation and a Monte-Carlo based radiative transfer model [Bernstein, 1988] that calculates radiative excitation and energy transfer between atmospheric layers.

The geometry module determines the species column densities, including aerosols/clouds, and the local density fluctuations of molecular species for each layer traversed by the user's requested paths. The multiple scattering sources are next extracted from a solution of the radiative transport equation for a vertical path through the atmospheric profile selected. The radiative transport module then calculates the mean radiance and local radiance fluctuations along each path for each molecular excited state, incorporating contributions from multiple scattering due to aerosols/clouds. The calculation is done on a line-by-line (LBL) basis with some approximations as will be described later in section 2.5. The non-stationary LOS radiance covariance is determined by performing LOS integrations over products of radiance fluctuation amplitude functions (defined in Section 2.4) and the local kinetic temperature covariance. It is pointed out that SAMM2 structure calculations only include fluctuations in densities of molecular species.

SAMM2 LBL capabilities extend those of FASCODE (Fast Atmospheric Signature Code) [Smith et al., 1978; Clough et al., 1981] into the NLTE regime at high altitudes. FASCODE is a first principles, line-by-line atmospheric radiance and transmittance code. FASCODE is the standard benchmark for atmospheric background codes based on band model approaches to radiation

transport. It is applicable from the visible to long wavelength infrared. It is generally used to calculate atmospheric radiance and path transmission at low altitudes, but can be used for non-equilibrium high altitude calculations if supplied with the appropriate vibrational level temperatures. SAMM2 directly calculates the non-equilibrium vibrationally excited populations in its chemical kinetics module.

SAMM2 line-by-line radiative transport, the Quasi line-By-Line (QBL) algorithm, is an approximate approach compared to FASCODE in the sense that in a given altitude layer a single normalized line shape is defined for each molecular isotope for all molecular transitions within a 0.5 cm^{-1} spectral bin. This means that line dependent Doppler and Lorentz widths in a spectral bin are approximated by (layer dependent) averaged values. In addition, true line-by-line calculations are performed near the center of each line, while averaged values are used for contributions from line tails. The SAMM2 RT algorithm is described in details in section 2.5.

A general discussion of atmospheric radiation and the important infrared-active molecules is given in the next section, with an overview of SAMM2 in Section 3. Sections 4 - 7 provide information on how to run SAMM2, input and output files, and the auxiliary programs for the input files. User instructions, supplemental information and a sample output are given in the appendices.

2. ATMOSPHERIC INFRARED RADIATION CONCEPTS

2.1 Local Thermodynamic Equilibrium vs. Non-Local Thermodynamic Equilibrium Conditions

Before discussing IR radiators in the atmosphere, we introduce the very important concept of non-local thermodynamic equilibrium (NLTE). Figure 1 shows the number of collisions a molecule suffers per second as a function of altitude. The relevant atmospheric properties (density, temperature, etc.) are taken from the U.S. Standard Atmosphere. The number of collisions decreases rapidly as a function of altitude [Sharma, 1988]. This fact influences the high-altitude IR airglow in a profound way. This can be seen as follows: At steady state the ratio of the density of a vibrationally excited species [M*] to the density of its ground state [M] is given by

$$[M*]/[M] = \frac{P_c + J}{L_c + A} , \qquad (1)$$

where P_c and L_c are the terms for production and loss, respectively, of M* due to collisions. J is the radiative pumping term due to absorption of radiation from earthshine, sunshine and the atmosphere, and A is the radiative loss term or the Einstein A Coefficient for spontaneous emission. At lower altitudes, the collisional production and loss processes are much faster than the radiative ones,

$$[M*]/[M] = P_c / L_c = Equilibrium \ Constant(K) , \qquad (2)$$

and local thermodynamic equilibrium (LTE) holds. Under these conditions IR airglow emitted by M* can be described by the Planck and Stephen-Boltzmann black body laws at the local thermal equilibrium temperature. When the radiative terms are not negligible compared to the collisional terms and Equation (2) can no longer be used to describe the situation, thermodynamic equilibrium no longer prevails. The situation is said to be in NLTE until the collision terms are much less than the radiative terms . A rule of thumb is that the radiation begins to deviate from LTE when there are less than a million collisions per radiative lifetime. The radiative lifetime of the $v = 1$ state of NO is about 0.1 s, so the 5.3 μm radiation from NO begins to deviate from equilibrium around 40 km altitude. This is an approximate but helpful rule which is applicable to species that are not produced by chemiluminescence or photodissociation. An exception to this rule of thumb is the 15 μm band of

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CO_2. Due to fast pumping during collisions with oxygen atoms [Sharma, 1988; Sharma and Wintersteiner, 1990], this mode stays in equilibrium up to above 100 km altitude [Rinsland *et al.*, 1992]. At very high altitudes the radiative pumping and loss terms J and A in Equation (1) are much larger than the collisional pumping and loss terms P_c and L_c. The ratio of the excited to ground state densities then becomes

$$[M^*]/[M] = J/A .$$

(3)

This situation is described as "radiative equilibrium". At altitudes greater than about 150 km the ratio of the densities of the CO_2 vibrational levels 01^101 and 00^001 is determined solely by the upwelling earthshine. The frequency of collisions is too small to have any impact and radiative equilibrium prevails.
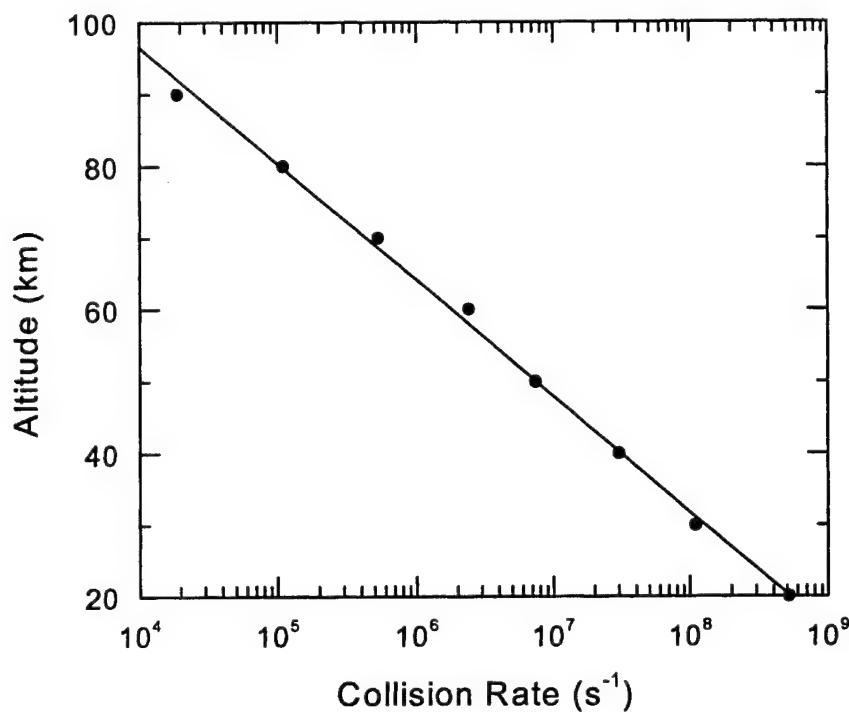
Figure 1. Dependence of the Atomic or Molecular Collision Rate on Altitude

The arguments cited above apply to stable species for which normally only the lowest vibrational level is populated and which may be excited by earthshine, sunshine, and collisions. They are not applicable to the species produced by chemiluminescence (OH and O_3) and by photodissociation (the singlet delta excited electronic state, $^1\Delta_g$, of O_2). In such cases the pumping and loss terms in

Equation (1) become more complicated because vibrationally excited levels may be populated by chemical reactions or by photodissociation, and these levels can influence the production or loss processes of other levels. We then have a number of coupled equations instead of the simple Equation (1). Nevertheless, Equation (1) nicely illustrates the basic points involved in calculating the ratio of the excited (upper) to ground (lower) state density.

2.2 Vibrational Temperature

At this point it is useful to introduce the concept of a vibrational temperature. This concept is based upon the experimental observation that translation to vibration (T - V) energy transfer rate coefficients are usually much smaller than translation to rotation (T - R) rates or the near resonant vibration to vibration (V - V) rates. Whereas T - V and T - R rates equilibrate translational degrees of freedom with vibrational and rotational degrees of freedom respectively, the V-V near resonant rates lead to the establishment of a Maxwell-Boltzmann distribution in a given vibrational manifold. We then have a situation where the translational and rotational degrees of freedom can be described by one temperature and the vibrational levels are described by an entirely different temperature. Of course two different vibrational manifolds in the same molecule may be described by two different vibrational temperatures. For example, the v_2 and v_3 vibrational fundamental states of CO_2 in NLTE situations invariably have different vibrational temperatures. If two vibrational modes are coupled by the Fermi or Dennison resonances, they may rapidly equilibrate and have the same vibrational temperatures. Again, the v_1 and v_2 modes of CO_2 coupled by their Fermi resonance are believed to have the same vibrational temperature. The vibrational temperature T_v is defined by the relation

$$T_v = c_2 E/[\ln(g_e n_l / g_l n_e)] ,$$

(4)

where g_e and g_l are the statistical weights of the excited and lower states, and n_e and n_l are their respective number densities (molec/cm^3). E is the vibrational spacing between the two levels in cm^{-1}, and $c_2 = 1.4388$ K/cm^{-1} is the second radiation constant. The temperature or population of the upper state is usually defined relative to the population of the ground state, that is, l is the ground state. It is clear from Equation (4) that T_v becomes equal to the translational (kinetic) temperature T when thermodynamic equilibrium prevails. Defining a vibrational temperature has proven to be a

useful concept because it not only indicates departure from equilibrium but also the extent of this departure.

Up to now the SAMM and SHARC models have assumed that rotational degrees of freedom are in equilibrium with translational motion. However, CIRRIS 1A results have shown that the rotational states of nighttime OH [Smith *et al.*, 1992] and daytime and aurorally produced NO [Joseph *et al.*, 1989; Sharma *et al.*, 1998] are not in equilibrium. Ongoing work is focusing on modeling these phenomena with a two-temperature rotational distribution, to be included in future releases of SAMM.

The lack of collisions leads to a departure from equilibrium (NLTE situations), but more frequent collisions do not guarantee thermodynamic equilibrium. This point is illustrated by the solar pumped airglow which, for bands like the 2.7 μm CO_2, can establish a steady state population of excited molecular levels higher than those given by LTE as far down as 50 km altitude.

2.3 Molecular Radiators

Currently SAMM2 supports the major isotope for NO, O_3, H_2O, CO, OH, CH_4, CO_2, HNO_3, N_2O, NO_2, SO_2, NH_3, and NO^+. Also the important minor isotopes of CO_2 and H_2O are included. We define natural conditions to be the quiescent and aurorally disturbed atmosphere. Atmospheric molecular emission in the infrared spectral region (1 to 40 μm) arises from either vibration-rotation (V-R) transitions of these molecules or from pure rotational transitions of OH and H_2O. Pure rotational transitions of NO, CO, and O_3 occur farther towards the red, around 100 μm, because these molecules have large moments of inertia; the pure rotational transitions for CO_2 are unallowed because it has no permanent dipole moment. The most abundant species, N_2 and O_2, have no IR vibration-rotation or pure rotational spectra because they have neither transitions nor permanent dipole moments.

The primary source of information about the intensity and location of the spectral lines is the HITRAN data tape [Rothman *et al.*, 1992; 1998]. It contains virtually all of the important lines for LTE conditions. Additional lines were added for NLTE transitions from the higher vibrational levels of $O_3(v_3)$ [Adler-Golden and Smith, 1990]. Supplementary data were also obtained for NO [Wintersteiner *et al.*, 1990], and for NO^+ [Winick *et al.*, 1987]. For OH, line locations and line strengths were based on a recent study [Goldman *et al.*, 1997]. The total intensity of the vibrational bands are given by their usual Einstein A coefficients, which are derived by a properly weighted average of the A coefficients of the individual V-R transitions [Winick *et al.*, 1987].

2.3.1 CO_2

Figure 2 shows the important CO_2 transitions observed in the infrared. There are three sets of strong transitions, which result in bands around 15.0, 4.3, and 2.7 μm. The relative strengths of the most important bands of these transitions are determined from their Einstein A coefficients. Some illustrative SAMM2 values for the most common isotope are given in Table 1.
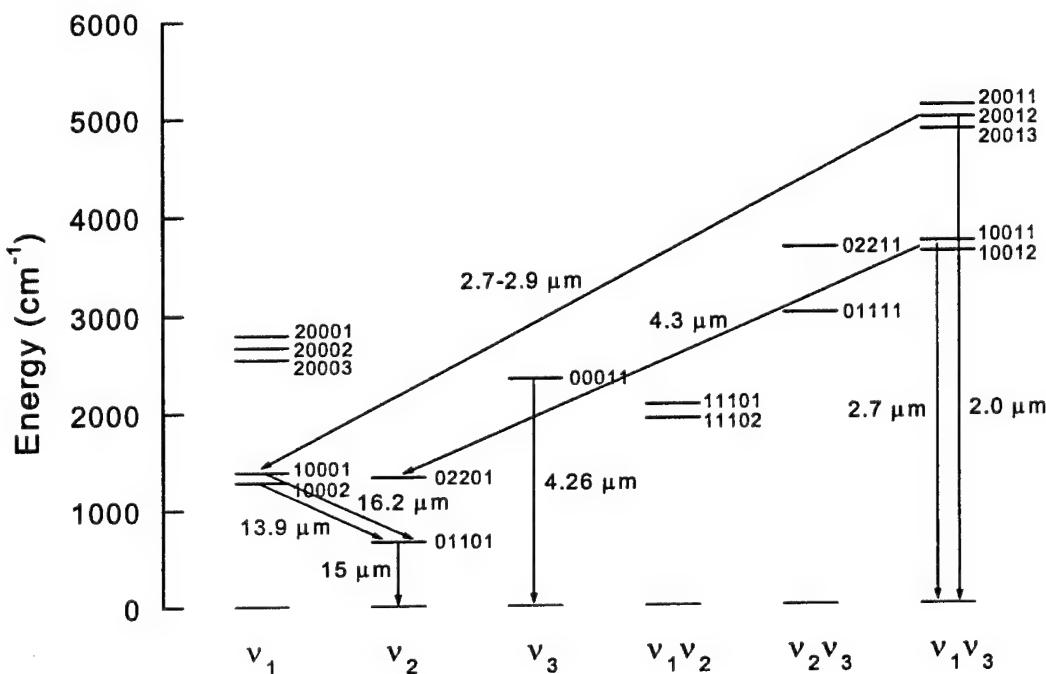
Figure 2. Important CO_2 Airglow Transitions and their Energy Levels

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Table 1. Illustrative Einstein A Coefficients for CO_2

TRANSITION	FREQUENCY (cm^{-1})	EINSTEIN A COEFFICIENT (s^{-1})
$10^002 \rightarrow 01^101$	618.	1.148
$01^101 \rightarrow 00^001$	667.4	1.500
$02^201 \rightarrow 01^101$	667.8	1.170
$10^001 \rightarrow 01^101$	721.	1.566
$00^011 \rightarrow 10^001$	961.	0.442
$00^011 \rightarrow 10^002$	1064.	0.467
$00^011 \rightarrow 00^001$	2349.	432.95
$10^012 \rightarrow 00^001$	3613.	11.15
$10^011 \rightarrow 00^001$	3715.	17.92

Around 15 μm, the bands result from a change of one quantum of bending mode v_2. These transitions are very prominent in the emission from the earth's atmosphere, and the sharp Q-branch can be clearly seen in spectra of the earth taken at spectral resolutions of a few wavenumbers from a balloon, rocket or satellite [Stair *et al.*, 1985; Wise *et al.*, 1995]. The reason for this is very simple. The spectrum of a 300 K blackbody peaks near 10 μm. Therefore, there are large numbers of 15 μm photons in the radiation, termed earthshine, emitted by the earth's atmosphere as well as by the earth itself. Since the 15 μm CO_2 band is very strong, its transitions to the ground state and low lying excited states are severely self-absorbed. This fact has important consequences for atmospheric radiation which we will point out as we go along. Similarly, solar radiation has negligible influence on the 15 μm radiation because of the small number of solar photons at this wavelength. The intensity of 15 μm radiation therefore shows no diurnal variation [Wise *et al.*, 1995]. This also indicates that population of the bending mode v_2 by relaxation or collisional deactivation of the solar pumped bands, e.g., 00^011, is unimportant. The second band, around 4.3 μm, arises from the emission of a quantum from the asymmetric stretch v_3. Because earthshine does not contain a strong 4.3 μm component, this band is much stronger during daytime. Solar radiation at 4.3 μm, 2.7 μm, 2.0 μm, and 1.6 μm is absorbed followed by a large probability of emission at 4.3 μm [Nebel *et al.*, 1994]. The probability of emission is largest at 4.3 μm because of the much larger Einstein A coefficients (Table 1) than those at 2.7 μm. The probability of re-emission at 2.0 and 1.6 μm is negligible because of their very small A coefficients. Transitions near 4.3 μm to the ground state and to the low lying excited states are also severely self-absorbed. The third band, around 2.7 μm, is due

to emission from the combination bands of $v_1 + v_3$. This emission, even more than the 4.3 μm component, is predominantly observed from the sunlit atmosphere.

In the aurorally dosed atmosphere a large amount of emission from the v_3 band of CO_2 around 4.3 μm is observed [Winick *et al.*, 1987]. This emission arises from the near-resonant transfer of vibrational energy from N_2 to the v_3 mode of CO_2. The nitrogen, in turn, is vibrationally populated by collisions with low energy secondary electrons. It takes a finite amount of time to transfer energy from N_2 to CO_2, and this time varies with altitude because of the density (see Figure 1). This CO_2 emission is called delayed emission as opposed to direct or prompt emission from an excited state of NO which is chemically created in an excited state and subsequently decays via photon emission.

Recent observations by the NASA TIMED/SABER instrument have indicated an enhanced CO_2 emission that is correlated to OH(v) emission, suggesting a role for OH(v) in indirectly exciting the v_3 mode of CO_2 by vibrational energy transfer from OH to N_2 to CO_2 [Lopez-Puertas *et al.*, 2004]. The mechanism of vibrational energy transfer between OH and N_2 is still however uncertain.

2.3.2 NO

Nitric oxide is a prominent radiator in the high altitude atmosphere. The 5.3 μm emission from its (1 - 0) vibrational transition is the most efficient atmospheric cooling agent between about 100 and 150 km altitude. This is because collisions between NO and atomic oxygen efficiently transfer translational energy into vibrational energy. The reverse V - T process has an almost gas kinetic cross-section at room temperature. The 5.3 μm emission from NO in the thermosphere is so bright that stratospheric limb radiance calculations that do not include NO emission in the thermosphere nor the excitation of these NO bands by thermospheric emission are likely to be incorrect.

In an aurorally dosed atmosphere, NO is also produced by the reaction between N atoms and O_2. The NO thus produced may be excited to vibrational levels as high as $v = 12$. The result of emission from high vibrational levels is that the fundamental band ($\Delta v = 1$) is spread towards longer (red) wavelengths. In contrast to the non-auroral atmosphere, overtone bands ($\Delta v = 2$) of NO around 2.7 μm are seen. A schematic diagram illustrating the atomic and molecular radiators produced in an auroral atmosphere is shown in Figure 3; further details are available elsewhere [O'Neil and Picard, 1985].
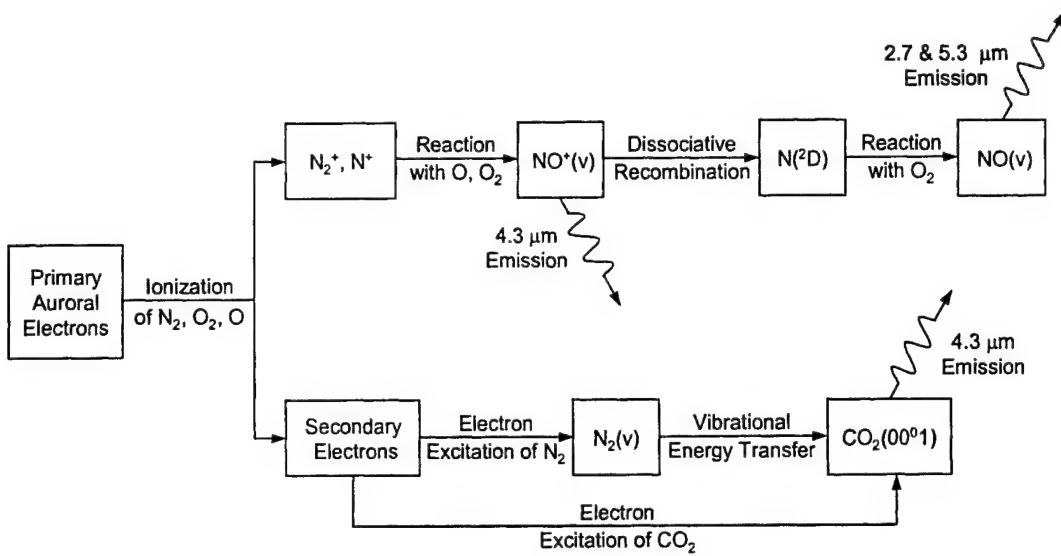
Figure 3. Illustrative Reaction Scheme Leading to Aurorally Enhanced Atmospheric IR Radiation at High Altitudes

2.3.3 O_3

The nonlinear triatomic molecule O_3 has three vibrational degrees of freedom. The vibrational mode v_1 at 1103 cm^{-1} has an Einstein A coefficient of about 0.5 s^{-1} compared to about 10 s^{-1} for the v_3 mode at 1042 cm^{-1} and about 0.08 s^{-1} for the v_2 mode at 701 cm^{-1}. Because of its much larger Einstein coefficient, emission from the v_3 mode is the dominant ozone emission observed from the earth's atmosphere. Ozone is formed by the reaction $O + O_2 + M \rightarrow O_3 + M$. It is well known that ozone is photodissociated by the ultraviolet component of solar radiation during the day. The same three body recombination reaction $O + O_2 + M \rightarrow O_3 + M$ regenerates ozone during nighttime. The ozone thus formed is in highly excited vibrational states. In the stratosphere, this newly formed ozone quickly loses its vibrational energy via collisions. However, because of the lower densities in the mesosphere, radiative processes, especially those involving the v_3 mode, become rapid enough so that emissions from excited vibrational levels are observed in the 10 - 13 μm region. Identification of levels responsible for this radiation is still not complete, and considerable work needs to be done before a complete model of ozone emission in the mesosphere can be constructed. Because of the decreasing total density, the three-body recombination process becomes slower in the thermosphere, and emission from ozone decreases rapidly.

2.3.4 H₂O

Figure 4 shows the three fundamental vibrational transitions of water vapor and the important combination and difference bands. Because of the prevailing temperatures, only transitions near 6.3 μm from thermally excited water molecules are observed in the nighttime atmosphere. Transitions near 2.7 μm and 4.85 μm originate from the vibration-rotation levels pumped by solar radiation. Vibration-rotation bands of water have a very complex rotational structure arising from the fact that water is an asymmetric top molecule with three different moments of inertia. Further, these moments of inertia are small and the fact that water has a large permanent dipole moment leads to its rich rotational spectrum in the 18 - 40 μm region. One possible source of excitation of these vibration-rotation levels is the accidental resonance of these levels with the nighttime emission from OH. Thus far, this source has not been shown to be the cause of any IR radiance due to the fast vibrational relaxation of water molecules
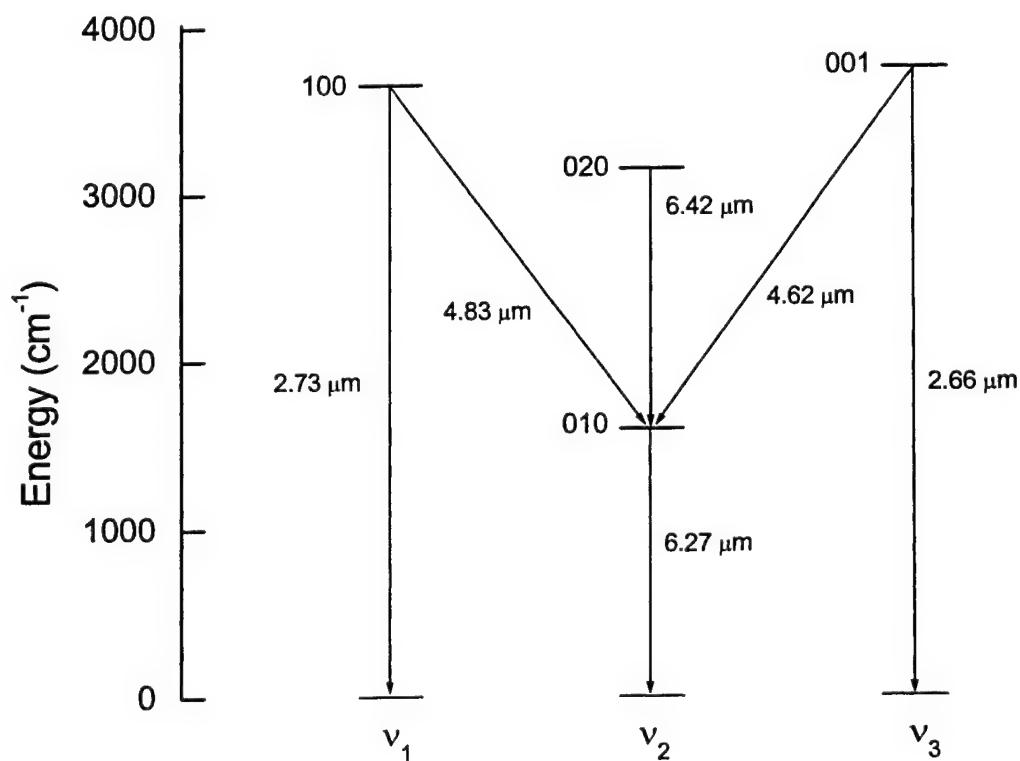
Figure 4. H₂O Transitions for the Lower Energy Levels that Contribute to Atmospheric IR Radiance at High Altitudes

2.3.5 CO

CO is another important atmospheric radiator because of its presence up to altitudes of 300 km. It is vibrationally excited by emission from the earth's surface and emission from the stratosphere during the night; during the day excitation by sunshine leads to further enhancement. CO vibrational excitation is not as closely tied to that of N2 as is that of asymmetric stretch v3 of CO2, because of its smaller rate for transfer of vibrational energy from N2 to CO. For this molecule, NLTE vibrational distributions exist at all altitudes. Recent comparisons with CIRRIS-1A data indicated that the CO radiance predicted by SAMM-2 is smaller than the observed radiance by a factor of almost two [Dothe *et al.*, 1996], suggesting an additional mechanism for vibrationally exciting CO.

2.3.6 OH

It is well established that the OH $\Delta v = 1$ and $\Delta v = 2$ emissions around 2.8 and 1.4 μm are important contributors to the near IR nighttime airglow in the 80-90 km altitude range. The OH radical is produced around 85 km primarily by the reaction [Sivjee and Hamwey, 1987; Adler-Golden, 1997]

$$H + O_3 \rightarrow OH + O_2 , \tag{5}$$

and possibly secondarily by the reaction

$$O + HO_2 \rightarrow OH + O_2 . \tag{6}$$

Both these processes produce vibrationally excited OH, with the first reaction producing excitations up to the ninth vibrational level. OH is one of very few molecules for which multiquantum radiative transitions are allowed. Thus the higher Δv transitions extend OH emissions all the way up to the visible spectral region. These vibrational transitions, for historical reasons, are called Meinel bands.

2.3.7 CH$_4$

A preliminary chemical kinetics model for CH$_4$ was developed for SHARC [Lang, 1991]. It contains the various vibrational excitation/deexcitation mechanisms and radiative relaxation processes. The CH$_4$ molecule as presently included in HITRAN possesses three major groups of

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bands around 2.3, 3.4, and 7 μm. The states associated with these transitions are shown in Figure 5. The vibrational state designation is adapted from HITRAN, where the first, second, forth, and sixth integers represent the v_1, v_2, v_3, and v_4 vibrations, respectively. The two low lying vibrational bends (v_2 and v_4) comprise transitions from Group 1 states to the ground state at 6.5 and 7.6 μm, respectively. Transitions from Group 2 to the ground state involve the symmetric and asymmetric stretches at 3.4 and 3.3 μm, as well as the first overtones of v_2 and v_4 and the $v_2 + v_4$ combination band. Of all these bands involving Group 2 states, the asymmetric stretch at 3.3 μm (v_3) is the strongest transition. Finally, the emissions near 2.3 μm are due to transitions from Group 3 states to the ground state (the $v_1 + v_4$, $v_3 + v_4$, and $v_2 + v_3$ combination bands), the strongest of which is the $v_1 + v_4$ band.
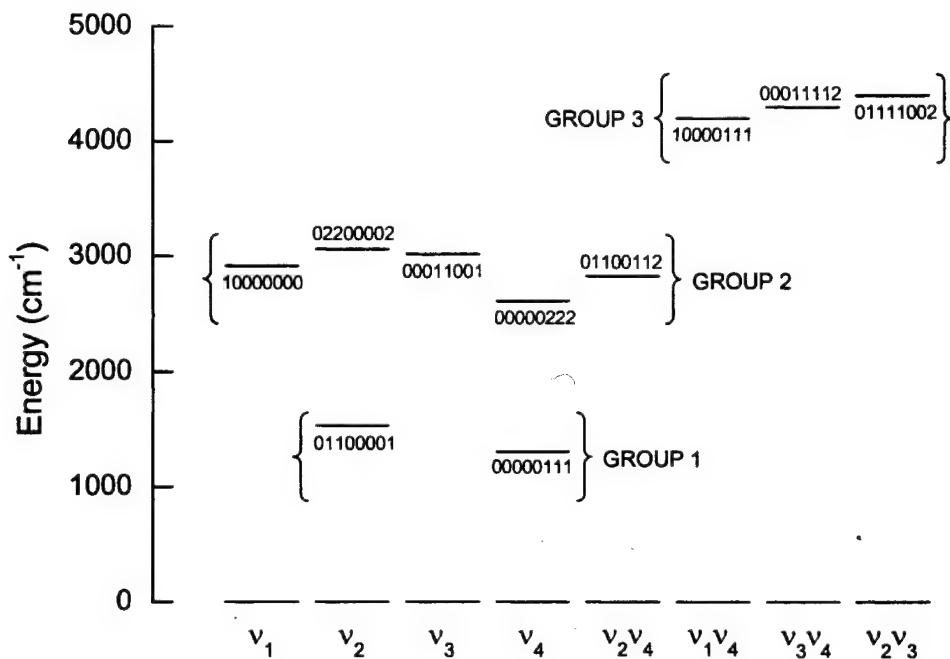
Figure 5. Vibrational Energy Level Diagram for CH_4

The most important energy transfer processes establishing the vibrational state populations are intermolecular vibrational-to-vibrational energy exchange between CH_4 vibrational states belonging to Groups 1, 2, and 3 with ambient O_2. A summary of the CH_4 bands included in SAMM2 are given in Table 2. Also shown are the strengths of the vibrational transitions as indicated by the Einstein A coefficients. CH_4 emission only makes a significant contribution to the short wavelength infrared (SWIR) emission during the daytime and to the long wavelength infrared (LWIR) during the daytime or nighttime in the lower mesosphere (around 50 km).

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Table 2. CH_4 Thermally Averaged Einstein A Coefficients

TRANSITION	FREQUENCY (cm^{-1})	EINSTEIN A COEFFICIENT (s^{-1})
00000111 → 00000000	1310.761	2.23
01100001 → 00000000	1533.337	0.054
00000202 → 00000000	2596.	0.0005
00000222 → 00000000	2612.	0.054
01100112 → 00000000	2830.	0.365
10000000 → 00000000	2917.	0.005
00011001 → 00000000	3018.921	24.43
02200002 → 00000000	3062.	0.086
10000111 → 00000000	4223.497	1.02
00011112 → 00000000	4320.	0.646
01111002 → 00000000	4540.	0.184
00011001 → 00000111	1708.160	0.650
00011112 → 00000111	3009.239	19.46
01111002 → 01100001	3006.663	13.43

2.3.8 HNO_3, N_2O, NO_2, SO_2, and NH_3

Emission from HNO_3, N_2O, NO_2, SO_2, and NH_3 occurs primarily from altitudes below approximately 30 km. The higher densities in the troposphere and lower stratosphere suggest that these molecules will be in LTE at the local atmospheric temperature, with the only exception being possible NLTE emission from $NO_2(v_3)$ in the stratosphere. Furthermore, since these molecules have complicated spectroscopic structure and chemical kinetics collision processes involving translational-to-vibrational and vibrational-to-vibrational energy exchange, the vibrational state populations are calculated assuming LTE conditions. Thus, the chemical kinetics mechanisms required for the high altitude NLTE species are not necessary for these molecules.

The major groups of bands for these molecules as presently included in HITRAN are as follows: HNO_3 5.8 μm (v_2), 7.6 μm (v_3, v_4) and 11 μm (v_5, $2v_9$) bands; N_2O 2.9 μm (v_1+v_3), 3.9 μm ($2v_1$), 4.5 μm (v_3), and 17 μm (v_2) bands; NO_2 6.2 μm (v_3) and 13 μm (v_2) bands; SO_2 7.3 μm (v_3) and 8.6 μm (v_1) bands; and NH_3 6.1 μm (v_4) and 10.5 μm (v_2) bands. In addition to the most important bands listed above, other minor bands included in HITRAN are currently supported by SAMM2.

2.4 Stochastic Radiance Structures

The calculation of infrared (IR) mean radiance, transmittance and their fluctuation statistics is important in many areas of atmospheric science, including the interpretation of satellite sensor measurements and for understanding the effects of turbulence structures on molecular excitation processes. The atmospheric infrared radiance fluctuations depend on fluctuations in atmospheric species number densities, vibrational state populations, and the kinetic temperatures along the sensor line-of-sight (LOS). The SAMM2 structure model predicts the two-dimensional spatial covariance function of the radiance for an image plane which is perpendicular to the LOS. The covariance function and its Fourier transform, the power spectral density (PSD), can be used directly in sensor models or in image synthesis models to create realizations of the predicted structure. The radiance statistics and images are non-stationary and are explicitly bandpass and sensor FOV dependent.

Fluctuations in atmospheric temperature and density have been measured directly using balloon, rocket, and satellite experiments. These experiments provide in-situ measurement of density, temperature and species concentrations. Ground based techniques used to determine atmospheric structure statistics include radar, lidar and airglow emission measurements. Taken together these measurements begin to provide the necessary structure statistics which characterize the atmosphere. Estimates of these quantities have been summarized in a 3-D non-stationary statistical model (NSS) [Strugala *et al.*, 1993]. The NSS model provides a covariance function, PSD description of atmospheric temperature and density fluctuations. Horizontal altitude layers are assumed to be isotropic and stationary. The vertical variations are non-stationary. Model parameters (variance, vertical correlation length, and horizontal correlation length) are described as a function of altitude. The NSS model assumes a 1-D PSD spectral slope of -2 for all altitudes. SAMM2 uses a form of the NSS model as its baseline temperature statistics model, but the user has the option to modify the spectral slope, variance, and vertical correlation lengths and horizontal correlation lengths. A more recent database of variance and horizontal correlation lengths was validated by MSX measurements. The MSX database is distributed with SAMM2 together with the older NSS database.

A simulation of the radiance fluctuations observed by a sensor array can be calculated by using a three-dimensional realization of the atmospheric temperature and density fluctuations and by intersecting a LOS for each pixel with the 3-D realization to determine the LOS radiance for each

pixel in the sensor [Brown, 1994]. Alternatively, the radiance statistics for the sensor FOV can be derived directly. The radiance statistical functions can be incorporated into sensor models, or image syntheses models, to create realizations of the radiance statistics. SAMM2 proceeds with the later approach although the former approach is being used to evaluate the algorithms. The radiance statistics predicted by SAMM2 explicitly include radiance fluctuation contributions along the entire LOS and not just the tangent point. The inputs to the calculation are altitude dependent temperature and density profiles, which can be obtained from the standard atmosphere generator code (SAG-2) [Shroll et al., 2003], the local temperature and density statistical quantities, an original and MSX-validated files for the NSS model are provided with SAMM2, and an atlas of molecular line parameters based on HITRAN-96 [Rothman et al., 1998]. The SAMM2 model calculates the non-stationary LOS radiance covariance by performing LOS integrations over the products of radiance fluctuation amplitude functions [Gruninger et al., 1994], and the local kinetic temperature covariance. A key quantity derived by the model is a LOS radiance variance distribution function which determines the contribution to radiance variance of each portion of the LOS. The radiance variance distribution function acts as a weighting function. It reveals contributions of temperature and density fluctuations to radiance variance along the LOS.

The radiance in a pixel of an image plane $L_{\Delta\lambda}(\mathbf{p})$ is given by

$$L_{\Delta\lambda}(\mathbf{p}) = \int d\lambda \int dr\, S(\mathbf{r}, \lambda) \partial\tau(r, \lambda)/\partial r \quad . \tag{7}$$

The quantity $S(\mathbf{r}, \lambda)$ is the emission source term at the wavelength, λ. The atmospheric transmittance, τ, along the LOS depends on the scalar distance r from the observer to the pixel and $\mathbf{p}$ is a vector in the sensor plane defining the pixel location. In the LTE approximation the source term is the Planck blackbody function at the local atmospheric gas kinetic temperature, T_k. In the NLTE regime the source term is dependent on the non-equilibrium number densities of the molecular states involved in the bandpass [Sundberg et al., 1994]. The populations of rotational states involved in the bandpass transitions are assumed to be in LTE. The vibrational states, j, are in NLTE. The dependence can be expressed in terms of vibrational state temperatures, T^j_{vib}. Implicit in Equation (7) is a sum over all species and their molecular states which emit in the bandpass, $\Delta\lambda$.

2.4.1 Vibrational State Temperature Fluctuations

The local temperature and density fluctuations induce fluctuations in the local vibrational state number densities. The influence of temperature and density enter into the chemical kinetic rate equations in a non-linear fashion. The collision rates are affected by temperature variations which alter rate constants and density variations which influence the number of collisions. The model predicts fluctuations in local vibrational state densities as a function of local temperature and density fluctuations. Nonlocal effects are not treated by the model. Temperature fluctuations cause two effects, a simple density expansion or compression which changes state populations induced by local heating or cooling respectively, and the adjustment of vibrational/rotational state populations due to the chemical kinetic mechanism. The latter effect can be expressed in terms of fluctuations in vibrational and rotational state temperatures. In SAMM2, the rotational states are considered to be LTE, so rotational temperatures and fluctuations map exactly with kinetic temperature fluctuation.

The fluctuation in local vibrational temperature for vibrational state, j, can be approximated as

$$\Delta T_{vib}^{j} = (\partial T_{vib}^{j}/\partial T_k)\Delta T_k + ... \tag{8}$$

The proportionality constants, $(\partial T_{vib}^{j}/\partial T_k)$, are strongly dependent on altitude and are also far from the LTE value of unity when NLTE effects are important.

As an example we illustrate the results of the NLTE kinetics model for determining the nighttime estimates of vibrational temperature and its response to temperature fluctuations for the CO_2 v_2 and v_3 fundamental transitions, see Figures 6 and 7. NLTE effects in vibrational state populations, and their linear response to fluctuations in temperature occurs for these states above 40 to 50 km. The NLTE effects in vibrational temperature is consistent with previous NLTE models and has been described previously [Lindquist, 1983]. Although vibrational temperature fluctuations have not been examined by other models, the fluctuations can be understood in terms of the same atmospheric processes determining the vibrational temperatures. In particular, the $CO_2(v_2)$ vibrational state involves collisional excitation by N_2 and O_2 which dominates below 50 km in the LTE regime, and diminishes in importance above 100 km. Radiative pumping is important above 50 km and dominates between 80 km and 100 km corresponding to the minimum in $\partial T_{vib}/\partial T_k$ around 80 km, as shown in Figure 6. Above 90 km, O atom excitation becomes increasingly important until ~250 km

where again radiative excitation dominates. The behavior of the $CO_2(v_3)$ state is quite different from $CO_2(v_2)$. $CO_2(v_3)$ is LTE up to approximately 30 km, and becomes completely dominated by radiative excitation by 50 km up to an altitude of 100 km. Although vibrational-to-vibrational energy transfer between CO_2 and N_2 is the most important mechanism between 110 and 170, there are not sufficient collisions to provide significant variations in the vibrational temperature in this altitude regime. Clearly, the altitude variations of the vibrational temperatures in response to temperature fluctuations will have a profound effect on the radiance fluctuations.
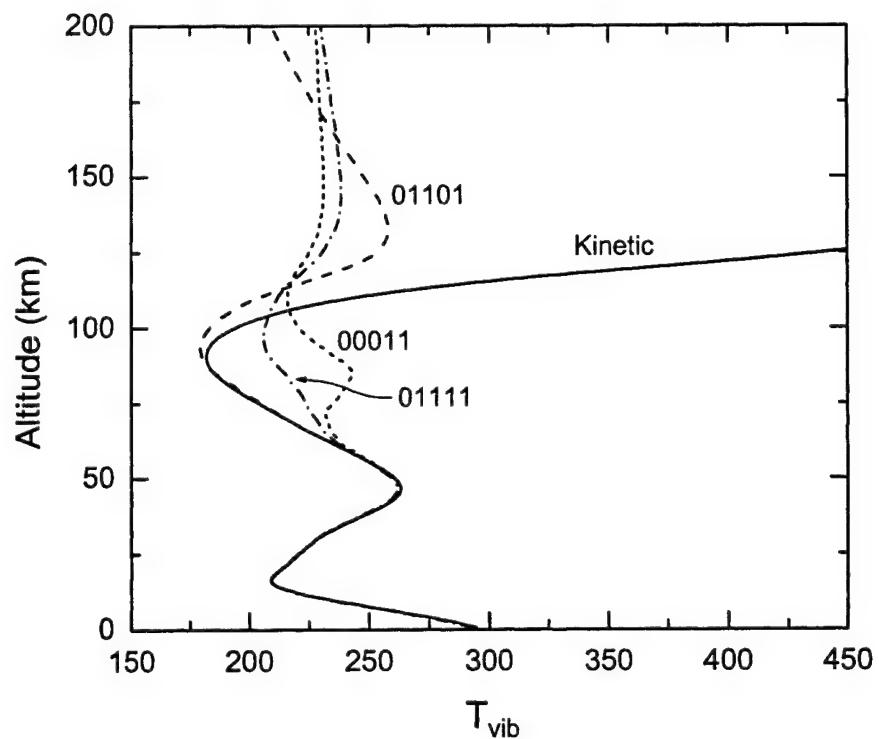
Figure 6. Atmospheric profile kinetic temperature and vibrational temperatures of selected states of CO_2 for nighttime conditions plotted as a function of altitude
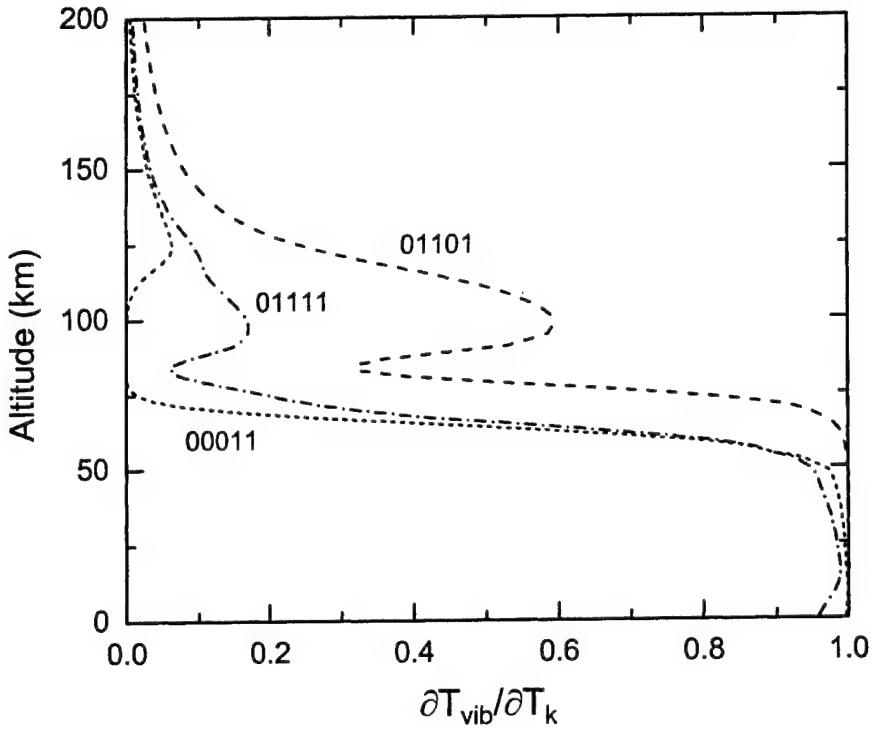
Figure 7. Partial derivatives of vibrational temperature with respect to kinetic temperature as a function of altitude for selected states of CO_2 for nighttime conditions

2.4.2 Radiance covariance

A fluctuation in radiance is approximated using the lead terms of a Taylor series expansion in terms of the vibrational state temperatures and the atmospheric temperature.

$$\Delta L_{\Delta\lambda}(\bar{p}) = \int dz \{ \sum_j F_{\Delta\lambda}^j(\bar{r}) \Delta T_{vib}^j + F_{\Delta\lambda}^0(\bar{r}) \Delta T_k \} + O[(\Delta T_k)^2] \quad . \tag{9}$$

The $F_{\Delta\lambda}^j$ and $F_{\Delta\lambda}^0$ are local LOS fluctuation amplitude functions. The radiance fluctuations induced by the rearrangement of population among the molecular vibrational states, j, is given by

$$F_{\Delta\lambda}^j(\bar{r}) = \int d\lambda \partial [S(\bar{r}, \lambda) \partial \tau(r, \lambda)/\partial r] / \partial T_{vib}^j \quad . \tag{10}$$

The radiance fluctuation induced by population shifts among rotational states, which are assumed to be in LTE, and the expansion or compression of the gas is given by

$$F_{\Delta\lambda}^0(\bar{r}) = \int d\lambda \, \partial [S(\bar{r}, \lambda) \partial \tau(r, \lambda)/\partial r] / \partial T_k \quad . \tag{11}$$

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Only the linear terms in Equations (8) and (9) are retained to make a direct estimate of the radiance statistics [Lindquist, 1983]. This approach is an extension of an LTE approximation used to determine atmospheric radiance statistics [Gruninger *et al.*, 1994]. The expression for a radiance fluctuation can be simplified in the linear approximation to

$$\Delta L_{\Delta\lambda}(\bar{p}) = \int dr \, F_{\Delta\lambda}(\bar{r}) \Delta T_k \quad , \tag{12}$$

where $F_{\Delta\lambda}(\bar{r})$ includes radiance fluctuation contributions from both vibrational state temperature fluctuations and kinetic temperature fluctuations

$$F_{\Delta\lambda}(\bar{r}) = \sum_j F_{\Delta\lambda}^j(\bar{r}) \partial T_{vib}^j / \partial T_k + F_{\Delta\lambda}^0(\bar{r}) \quad . \tag{13}$$

The fluctuation amplitude defined by Equation (13) is a linear response model for radiance fluctuations in terms of gas kinetic temperature fluctuations. This model can be coupled with a statistical model for non-stationary atmospheric temperature fluctuations to obtain a statistical non-stationary description of radiance fluctuations.

The radiance covariance $Cov_L(\bar{p}_1, \bar{p}_2)$, where $\bar{p}_1$ corresponds to point 1, and $\bar{p}_2$ to point 2, in the sensor plane, can be expressed as

$$Cov_L(\bar{p}_1, \bar{p}_2) = E[\Delta L_{\Delta\lambda}(\bar{p}_1) \Delta L_{\Delta\lambda}(\bar{p}_2)] \quad , \tag{14}$$

where E is the expectation value. This geometry is illustrated in Figure 7. Substituting Equation (12) into Equation (14) yields

$$Cov_L(\bar{p}_1, \bar{p}_2) = \int dr_1 \int dr_2 F_{\Delta\lambda}(\bar{r}_1) F_{\Delta\lambda}(\bar{r}_2) Cov_T(\bar{r}_1, \bar{r}_2) \quad . \tag{15}$$

The radiance variance, $\sigma^2(\bar{r})$, is determined by setting $\bar{p}_1 = \bar{p}_2$ in Equation (15) so there is zero lag

$$\sigma_L^2(\bar{p}) = \int dr \int dr' F_{\Delta\lambda}(\bar{r}) F_{\Delta\lambda}(\bar{r}') Cov_T(\bar{r}, \bar{r}') \quad . \tag{16}$$

Equation (16) shows the dependence of the radiance variance on the atmospheric temperature covariance along the LOS direction. Integration over one of the variables in Equation (16) leads to a LOS variance distribution function, or weighting function, $w_{\Delta\lambda}(\bar{r})$

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$$\sigma_L^2(\bar{p}) = \int dr \, w_{\Delta\lambda}(\bar{r}) \tag{17}$$

where

$$w_{\Delta\lambda}(\bar{r}) = \int dr' \, F(\bar{r}')F(\bar{r})Cov_T(\bar{r},\bar{r}') \quad . \tag{18}$$

The variance distribution function determines how contributions to the radiance structure are distributed along the LOS through the atmosphere. The area under the distribution function curve is the radiance variance at the pixel location $\bar{p}_1$. The variance distribution function, $w_{\Delta\lambda}$, is evaluated numerically.

The role of the spatial statistics of the 3-D temperature structures is revealed through the radiance variance distribution function. The temperature correlation length along the LOS direction controls the extent to which temperature fluctuations are averaged by LOS radiation transport. The temperature correlation lengths perpendicular to the LOS determine the spatial radiance statistics in the sensor plane. The statistical properties of the radiance fluctuations such as correlation angles or lengths can be determined directly from the covariance function, or they can be approximated using the variance distribution function [Sundberg *et al.*, 1994].

2.4.3 Image Synthesis

The bandpass dependent statistics of the radiance fluctuations, can be input into a model for synthesizing images. The radiance statistics are non-stationary. This requires an image generator which can deal with spatially varying statistics. Such an image generator has been recently described by Brown et al. [1997]. One of their methods uses a nonlinear "stretched-space" mapping transformation to produce a nonstationary synthetic stochastic realization of the radiance statistics generated by SAMM2. A second method is to generate a 3-D grid of temperature fluctuations and propagate lines-of-sight through the grid using SAMM2 3-D statistics. A third technique relies upon an adaptive autoregressive algorithm to compute spatial radiance fluctuations at the sensor plane from the SAMM2 2-D radiance statistics. In Figure 8 we show a sample image for an MWIR CO_2 band pass which was generated using the technique of Brown and Grossbard.

22
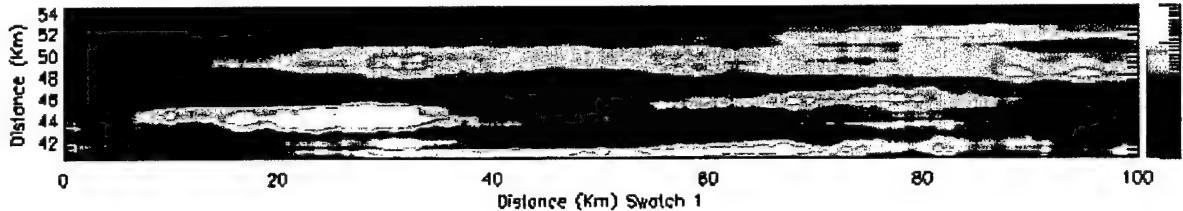
Figure 8. Clutter image for CO2 MWIR Bandpass for Nighttime Conditions

2.5 Radiation Transport (RT) Algorithm

In SAMM2, spectral emission, I_v^{em} (R), is calculated as a LOS (line-of-sight) integral of the product of path transmittance and emitted radiation:

$$I_v^{em}(R) = \int_0^R e^{-\tau_v(r)} \sum_i J_{vi}(r) \, k_{vi}^a(r) \, \rho_i(r) \, dr \quad , \tag{19}$$

where R is the LOS (line-of-sight) distance;

i is the species (molecular or particle) index;

v is the spectral frequency;

$\tau_v(r)$ is the extinction optical depth;

$J_{vi}(r)$ is the emission source;

$k^a{}_{vi}(r)$ is the absorption cross-section; and

$\rho_i(r)$ is the molecular or particle density.

If the path terminates at a hard body such as the earth, a surface emission term is included.

The extinction optical depth, τ_v (r), is the LOS integral of extinction (absorption + scattering) cross-section, $k^x{}_{vi}$ (r), and local density products:

$$\tau_v(r) = \int_0^r \left(\sum_i k_{vi}^x(r') \, \rho_i(r') \right) dr' \quad . \tag{20}$$

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The emission source, $J_{vi}(r)$, may be particle or molecular. Particle emission is thermal. Molecular emission is thermal under LTE (local thermodynamic equilibrium) conditions, but not under NLTE (non-LTE) conditions:

$$J_{vL}(r) = \frac{c_1 v^3}{\pi} \left(\frac{\rho_L'(r)/g_L'}{\rho_L''(r)/g_L'' - \rho_L'(r)/g_L'} \right) \quad (NLTE)$$

$$= B_v(T(r)) \quad (LTE)$$

(21)

where $\rho_L'(r)$ is the molecular upper state number density;

$\rho_L''(r)$ is the molecular lower state number density;

g_L' is the molecular upper state statistical weight;

g_L'' is the molecular lower state statistical weight;

c_1 is the first radiation constant ($2\pi\, h\, c^2 = 3.7418 \times 10^{-12}$ W cm^2);

$T(r)$ is the LTE (translational) temperature; and

$B_v(T)$ is the Planck function at temperature T and spectral frequency v.

Here the index i has been replaced by index L to emphasize that the attenuation source is molecular line absorption. Since the LTE emission source is species independent, monochromatic emission can be computed directly from path extinction and absorption optical depths given the temperature profile. For the NLTE (non-LTE), it is necessary to couple the absorption source and optical depth terms together LBL (line-by-line).

Molecular line absorption is partitioned into four regions: line center, local line tails, extended line tails, and continua.

$$\sum_L = \sum_{centers < 2\Delta v} + \sum_{tails < 2\Delta v} + \sum_{tails > 2\Delta v} + \sum_{continua}$$

(22)

The precise definition of each region is illustrated by the figure below.
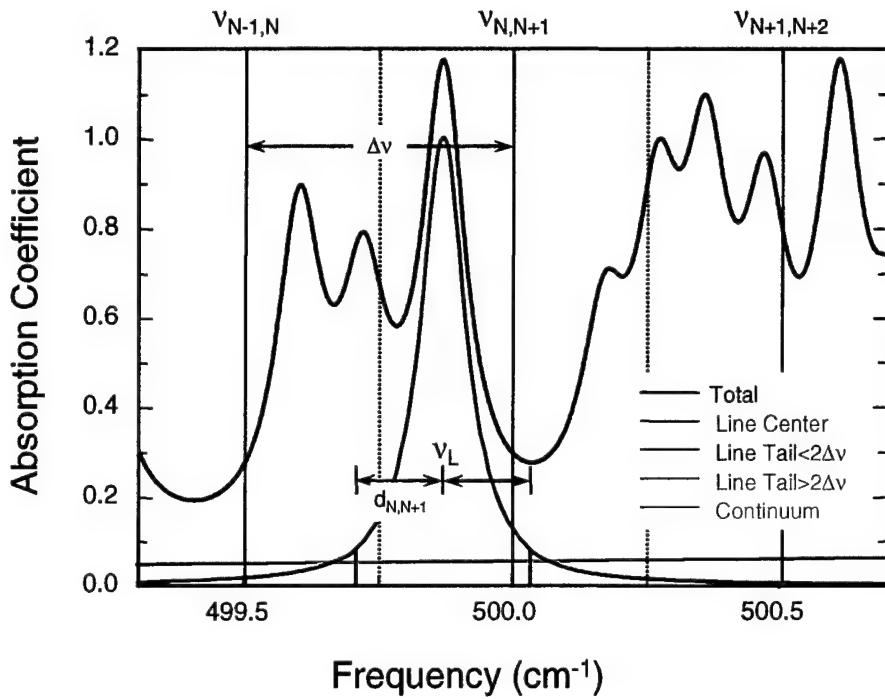
Figure 9. Definition of the spectral regions for computing the molecular absorption coefficient.

For each line in the SAMM2 lines file, line center absorption is calculated at high spectral resolution in the spectral bin ($\Delta v = \frac{1}{2}$ cm-1) containing the line and, if necessary, in its nearest neighbor spectral bin. Consider a line with transition frequency v_L. Its absorption coefficient within the calculational bin of width δv (= 0.001 cm-1) centered at frequency v is the product of the temperature-dependent line strength, $S_L(T, T^j_{vib})$, and the normalized Voigt (combined Doppler-Lorentz) line shape, $f_{\gamma c,\gamma d}(v - v_L)$:

$$k^a_{v_L}(line\ center) = \frac{S_L(T,T^j_{vib})}{\delta v} \int\limits_{v-\delta v/2}^{v+\delta v/2} f_{\gamma_c,\gamma_d}(v' - v_L)\, dv'$$

$$\approx S_L(T,T^j_{vib})\, f_{\gamma_c,\gamma_d}(v - v_L) \tag{23}$$

The molecular line strength is a function of total and state molecular number densities, which in turn depend on translational (assumed equal to rotational) and vibrational temperatures:

Here, $B_{\rho''\rho'}$ is the temperature-independent Einstein coefficient for induced absorption, retrieved from the HITRAN database.

Local linetail contributions to the current ($\Delta v = \frac{1}{2}$ cm^{-1}) spectral bin, from lines located less than 2 Δv away (i.e., $\pm \Delta v$ from the center of the bin), are modeled as a spectrally constant baseline continuum within each interval. For a line with transition frequency v_L located nearest to the spectral boundary $v_{N,N+1}$ (see Figure 9), the local line tail contribution to spectral bin N is

$$
k_{v\,L}^a \; (\text{local line tail}) \; = \; \frac{S_L}{\max\{v_{min,L}, v_{N-1,N}\} - v_{N-1,N}} \; \int_{v_{N-1,N}}^{\max\{v_{min,L}, v_{N-1,N}\}} f_{\gamma_c, \gamma_d}(v' - v_L)\, dv'
$$

(25)

$$
+ \; \frac{S_L}{v_{N,N+1} - \min\{v_{max,L}, v_{N,N+1}\}} \; \int_{\min\{v_{max,L}, v_{N,N+1}\}}^{v_{N,N+1}} f_{\gamma_c, \gamma_d}(v' - v_L)\, dv'
$$

where $v_{min,L} = v_L - d_{N,N+1}$, $v_{max,L} = v_L + d_{N,N+1}$, $d_{N,N+1}$ is a line spacing parameter derived from HITRAN.

Extended Lorentzian line tails contributions to the current ($\Delta v = \frac{1}{2}$ cm^{-1}) spectral bin, from lines located $> 2\ \Delta v$ and < 25 cm^{-1} away from the bin center (see Figure 9), are obtained from pre-summed, LTE values stored in the LTE tails data file as described later in Section 6.5.2.

Absorption coefficient tail contributions from beyond 25 cm^{-1} from line center are included as LTE continua for CO_2, H_2O, O_3, NO_2, SO_2, O_2 and N_2. The CO_2 continuum has of the form

$$
k_{v,T}^a (CO_2 \; continuum) \; = \; v \left(\frac{1 - e^{-c_2 v / T}}{1 + e^{-c_2 v / T}} \right) C_v^{CO2} \left(\frac{T_{ref}}{T} \frac{P}{P_{ref}} \right) \quad ,
$$

(26)

where c_2 is the second radiation constant (h c / k = 1.4388 cm K) and C_v^{CO2} is a spectral coefficient. In FASCODE, C_v^{CO2} is stored in block data, tabulated at 10 cm^{-1} spectral resolution between 0 and 10,000 cm^{-1}. MODTRAN instead incorporates the CO_2 continua data directly into its extended line tail data. This latter approach has been adopted for SAMM2 for greater computational efficiency.

The H_2O continuum model is similar to the CO_2 model except that contributions from water self broadening are separated out and temperature dependent between 260 and 296 K

$$k_{v,T}^{a}(H_2O\,continuum) \quad = \quad v\left(\frac{1-e^{-c_2v/T}}{1+e^{-c_2v/T}}\right)*$$

$$\left\{C_{v,foreign}^{H2O}\left(\rho_{TOT}-\rho_{H2O}\right)+\left[C_{v,self\,260K}^{H2O}+\left(\frac{T_{H2O}-260K}{296K-260K}\right)\left(C_{v,self\,296K}^{H2O}-C_{v,self\,260K}^{H2O}\right)\right]\rho_{H2O}\right\} \quad . \tag{27}$$

The temperature T_{H2O} is water density weighted average temperature for a path segment along the LOS. The H_2O continuum coefficients cannot be incorporated into the extended line tail parameters because of the separation of the self- and foreign-broadened terms. Instead, the H_2O continuum has been directly integrated into SAMM2. The SAMM2 continuum coefficients are taken from MODTRAN4.

2.6 Cloud and Aerosol Multiple Scattering

SAMM2 includes aerosol and cloud models from MODTRAN4. NOVAM models are not included in the current version. Scattering contributions are computed, as in MODTRAN, using either the (two-flux) ISAACS model or the DISORT (Discrete Ordinate Radiation Transport) algorithm. Because MODTRAN and SHARC use different altitude grids (a finer grid in MODTRAN for the lowest altitudes near the ground while in SHARC a finer grid for the higher altitudes), a layer merging algorithm is used in SAMM2 to combine the two grids. First, in order to compute the multiple scattering (MS) source functions, the atmospheric profiles obtained for the SHARC altitude grid are mapped into the MODTRAN grid and combined with the aerosols/clouds densities. Then, after the MS source functions have been calculated in the MODTRAN grid, they are remapped into the SHARC grid for the radiative transport calculation.

Some features of MODTRAN are not currently available in this version of SAMM2. These include NOVAM models, correlated-k RT capability, bandpass instrumental response functions, scaled DISORT MS (Multiple Scattering) contributions, option for separate output of solar irradiance

contribution, capability of scaling aerosols and clouds concentrations, water and ozone densities, moving locations of clouds, adding custom (user specified) species, and predicting adjacency effects (contributions to radiance from considered pixel from pixels adjacent to it).

3. OVERVIEW OF SAMM2

SAMM2 calculates atmospheric radiance, transmittance and radiance structure statistics under both LTE and NLTE conditions for paths from the ground to 300 km. The user has considerable latitude to modify the atmospheric model being used. The modifications can be to the density profiles of species, statistical properties of the atmospheric temperature profile, and to the kinetics governing the chemical and radiative processes undergone by those species. These modifications are achieved by changes to various data files, while leaving the code itself unchanged.

The spectroscopic states and bands for each radiating atmospheric species and the differential equations representing the kinetic scheme governing the NLTE energy level populations are defined in external data files rather than built into the code. Also defined via data files are the vertical concentration profiles of all atmospheric constituents, including those of N_2 and O, which do not contribute directly to the IR radiation but serve as collision partners in the kinetic schemes. Specific local atmospheric environments can be specified through region definitions. Diurnal characteristics within a region can be specified through multiple vertical concentration profiles which can be supplied by the user or generated for specific geomagnetic conditions by SAG-2, the SHARC/SAMM Atmospheric Generator [Shroll et al., 2003].

For calculations involving the solar terminator, the attenuation of solar irradiance by aerosols must be estimated. For each radiating species, absorption parameters for the lower atmosphere aerosols have been calculated with MODTRAN and are stored in a file.

The statistical properties for the atmospheric temperature are stored in an altitude dependent file which can be modified by the user. Two files are provided with SAMM2, one based on the NSS model, while the other is based on more recent analysis of MSX data.

Finally, for the LOS calculations of radiation transport, once the NLTE populations have been determined, spectral parameters for all individual radiating lines are obtained from a modified-HITRAN data file.

The input files, which define the species' spectroscopic states and bands and the lower-atmosphere filtering, are written in a simple ASCII format and read directly by SAMM2. The

kinetics scheme for a particular radiator is also written in an ASCII format, but it must be translated into a form accessible to the CHEMKIN-derived [Kee *et al.*, 1980] AMBIENT module using it. The ASCII representation of the kinetic differential equations closely follows the notation used by chemical kineticists for, say, publications or calculations on paper; explicit FORTRAN statements do not appear. The translation is accomplished by a separate, auxiliary program called the INTERPRETER. This program, discussed in more detail in Section 7, reads the ASCII kinetics file and produces an ASCII "linking" file which provides the required information for the AMBIENT module.

In addition to performing calculations for a single line-of-sight, SAMM2 is designed to enable simulation of a two-dimensional scene as recorded by a sensor. For that reason, the user has the choice of performing SAMM2 calculations either for a single line-of-sight or for a series of lines-of-sight encompassing the entire scene during a single execution of the code. The user is offered several ways for specifying lines-of-sight appropriate for a scene. One way, for example, is to specify the two tangent heights delimiting the field-of-view of the sensor, and the number of lines-of-sight to be equally spaced within the FOV. This assumes horizontal isotropy as is the case with the current radiance structures model. A future release will treat non-isotropy in the horizontal direction.

There are two different modes for running SAMM2; they are

- interactive with input menus, or

- batch submission with a previously completed input file.

After interactively preparing the input file, the user has the option to proceed directly to execution or to exit and restart the code interactively or as a batch run. Both methods provide SAMM2 with an input file stating the exact calculation to be performed.

In the first mode, the user can specify the problem by starting SAMM2 in its interactive mode. All input requirements are solicited from the user through a series of screen menus. All input is checked for consistency during the interactive session, and at the end of the session a new SAMM2.INP file is created containing the verified inputs.

The SAMM2 interactive input module presents the user with a sequence of menus for processing SAMM2.INP input files. The SAMM2.INP file contains the calculation specific information. Separate menus allow the user to define the atmospheric regions which may be encountered by a LOS, in terms of atmospheric profiles, temperature statistics, solar angles, molecular radiators, local region geometry, and local ambient and auroral environments. Additional menus allow the user to select specific LOS geometries, spectral intervals and resolution. The interactive input module provides additional menus for input file name and directory selections. All inputs are checked for validity and consistency so that run time errors can be minimized. Detected errors and inconsistencies are reported to the user during the interactive session so that the inputs can be repaired during the session. The existence of user selected directories and input files are also verified during the interactive session.

The second mode for running SAMM2 is batch submission with a previously created SAMM2.INP file. In batch mode, the SAMM2.INP files that are listed in the SAMM2.JOBS file are read by SAMM2 and checked for errors and inconsistencies before calculations are performed. If input errors or inconsistencies are detected the problems are reported in the SAMM2.LOG file and execution is terminated before calculations are initiated.

3.1 Calculational Flow

The first step in running SAMM2 is to insure that all needed files are available. If the program is being used as shipped, the user only needs to generate the binary linking files, generate the binary file of spectral lines, create accessible directories, and place the data files in them. If modifications to the kinetics, states, bands, or atmospheric profile files are required, the user must take care to insure that the files for each radiator remain mutually consistent, as discussed in Section 7. Changes in the kinetics scheme require running the INTERPRETER program to generate the linking file for SAMM2.

The calculational sequence in SAMM2 is shown schematically in Figure 10.
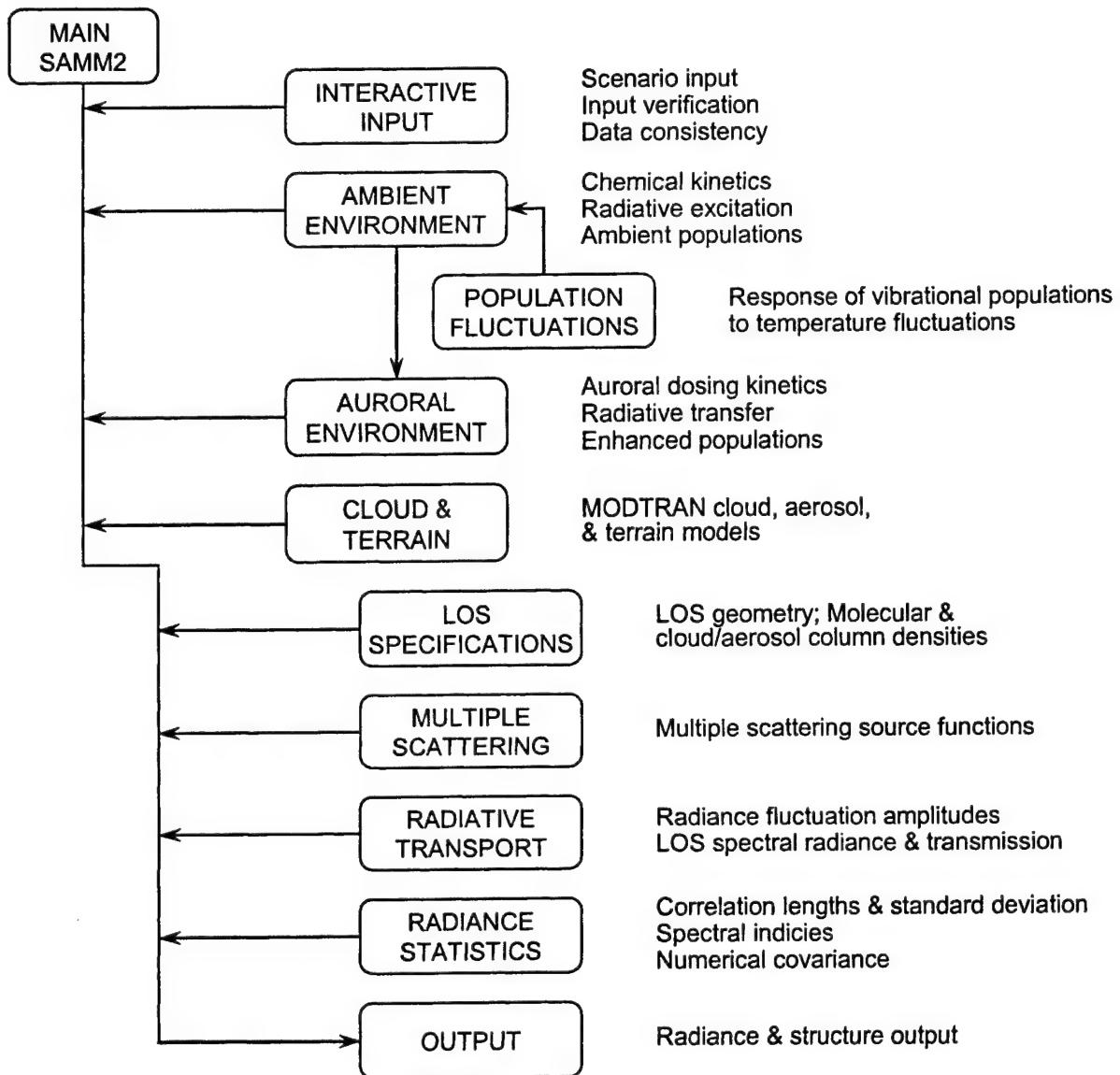
Figure 10. Calculational sequence for SAMM2.

The main routine acts as a driver. First it calls a set of routines which are used to define and verify problem specific inputs, then it calls the remaining routines to carry out the calculations and store the results.

The ambient population routines calculate the various molecular state populations for every atmosphere specified by the user. Each region may have from one to seven atmospheres. If an auroral calculation is requested, the auroral module then calculates population enhancements for those regions designated as auroral. If atmospheric structure is requested, excited state number

density fluctuation terms are calculated for use in the radiance calculation. Auroral regions can not be used in structure calculations, since SAMM2 does not include the appropriate auroral structure models. The LOS specification module and the radiation transport module then determine the LOS and the atmospheric radiance and transmission expected to be observed along that LOS, and the results are output for later examination.

The ambient atmospheric chemistry module calculates altitude population and population fluctuation profiles for the various molecular vibrational states. These calculations can be lengthy, and it must be emphasized that these profiles should be re-used when different LOS paths are being calculated for the same atmospheric conditions. The ambient chemistry module includes two components, a chemical kinetics module (CHEMKIN) and a radiative transfer module (NEMESIS). Together they calculate the NLTE populations and population fluctuations for the various molecular excited and ground states. CHEMKIN calculates the steady-state excitation due to chemical reactions, energy transfer processes, and solar and earthshine pumping. NEMESIS then calculates changes in the excited-state populations due to radiative transfer between molecules in the entire atmosphere. The auroral chemistry module then calculates the auroral enhancement of these ambient populations. This module uses a time-dependent chemical kinetics module (CHEMKIN) and a simplified radiative transfer model based on Kumer's Q_w approximation to calculate the radiative transfer within the aurora [Kumer and James, 1974].

The cloud and aerosol physical and optical properties are provided by the MODTRAN4 databases. The surface reflectance information is again based on MODTRAN4 reflectance models and databases.

The LOS specification module divides the LOS into small segments with constant properties. For each segment it determines the local atmospheric temperature, pressure, and the mean and fluctuations associated with the molecular state column densities of each excited state. The density profiles calculated by the ambient and auroral modules are used to determine these LOS column densities.

To account for multiple scattering in SAMM2, multiple scattering (MS) source functions are added to the usual SHARC-4 NLTE sources. MS effects are then fully included by combining these

MS source functions with total optical depths that include all particle extinction properties. This approach retains consistency with the spectral radiance routines in previous SHARC versions, although SAMM2 is now a line by line code. The NLTE MS source is computed by subtracting the Black Body source from the LTE source function obtained from MODTRAN4, and adding to it the SHARC-4 NLTE source.

The radiation transport module utilizes the information provided by the LOS specification module along with a molecular spectroscopic database to determine the LOS spectral radiance. It uses an effective LBL approach in that the total path radiance from each spectral line using a Voigt lineshape is calculated. These line radiances are obtained at high spectral resolution (0.001 cm^{-1}) and then degraded by a triangular slit function, whose spectral width is defined by the spectral increment of the calculation. If the atmospheric structure option is used, the LOS and bandpass dependent radiance statistics are also determined.

3.2 Principal Features of SAMM2

3.2.1 MAIN Routine

The SAMM2 MAIN module has a brief main program which simply reads the SAMM2.JOBS file and passes the name of the input file, for example SAMM2.INP, to an extensive first-level routine which carries out necessary sequence of major module calls, required to perform the tasks specified in the input.

Usually the user will place an input file (say SAMM2.INP), set for interactive execution, in the same directory as SAMM2. The numeral "1" in the first non-comment input line specifies interactive operation. The numeral "0" in the first non-comment input line specifies batch operation. If no SAMM2.INP file exists, a default interactive-mode file is created by SAMM2, and an interactive session is initiated.

3.2.2 INTERACTIVE INPUT Routines

When started, SAMM2 reads the SAMM2.JOBS file and calls the input module first, regardless of whether the mode is interactive or batch. If the SAMM2.INP file is marked as interactive, the

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module will let the user create a new SAMM2.INP file. The user defines parameters by making choices from a tree-structured series of menus; menu choices include either parameter definitions or lower-level menus. Initial parameter settings are determined by the current SAMM2.INP file, which is read in before the first menu is presented to the user. The menu structure is discussed in more detail in Subsection 4.2 below. Again, the fundamental aspects of atmospheric structure and chemistry are defined in the external data files; the INPUT parameters then tell SAMM2 what calculation is to be performed. The user selects ambient and auroral regions, temperature structure statistics, LOS specifics, molecular radiators, spectral intervals, and spectral resolution. The module also allows the user to customize the code for a particular computing environment through selection of directories for various input/output files and naming conventions for kinetics input files.

After the user has completed the inputs for the calculation, execution can be continued from the main menu. However, the more common choice is to exit the interactive session and have SAMM2 write a SAMM2.INP (the name of the file can be user defined – say TEST13.INP) that has been set for batch execution (numeral "0" in the first non-comment line).

In either mode, the code will execute, write its several output files, and stop with no further input from the user.

The LOS inputs allow arbitrary paths above 0 km altitude. There are three general categories of LOS's supported by SAMM2:

- observer to a specified source location
- observer to space (the default altitude for space is the top of the defined atmospheric profile)
- limb viewing (space to space through the limb)

The user also has various options within these categories. The input module computes a uniform set of path quantities from the user's parameter set. Parameters for these options are discussed in Subsection 4.3.3 below. A curved-earth geometry is used for all LOS path calculations. Atmospheric refraction is included for all paths, regardless of LOS options. See Subsection 4.3.4 for further details.

In addition to accepting input interactively, all intersections of the input LOS with atmospheric regions and solar zenith variations along the LOS are determined and displayed on the screen. This allows the user to assess the appropriateness of the LOS selection prior to program execution. All inputs are checked for consistency and for being within the bounds set by the program. All specified input and output files and directories are checked for their existence, status (new or old) and accessibility. All inconsistencies and file specification errors are reported to the user prior to exiting the interactive mode so that repairs can be made during the interactive session. When the batch option has been selected the input file SAMM2.INP is read and this module performs all checks for input consistency and file specification errors. If inconsistencies or errors are found, an explanation of the inconsistency is written to the SAMM2.LOG (note that the prefix name, SAMM2, can be user specified) file, and execution is terminated. If no inconsistencies or errors are found, the SAMM2 input file is updated with the new LOS information.

3.2.3 The Ambient Population Routines

This group of routines has two components, CHEMKIN and NEMESIS. CHEMKIN calculates excited state populations within each atmospheric layer (defined by the boundaries input from atmosphere input file), while NEMESIS calculates the radiative interaction between states in different atmospheric layers. The calculation is an iterative process; CHEMKIN starts, NEMESIS radiatively modifies some populations, and then CHEMKIN recalculates the state populations. The first component, CHEMKIN, computes the steady-state number densities of vibrationally excited atmospheric species from a set of chemical kinetics/reaction mechanisms for each atmospheric layer. Its subroutines are based on those in the Sandia Livermore CHEMKIN package [Kee *et al.*, 1980].

The SAMM2 CHEMKIN module computes the steady-state number densities of vibrationally excited atmospheric species from the set of chemical kinetics/reaction mechanisms prepared by the INTERPRETER. The chemical kinetics equations are solved for the particular atmospheric conditions selected by the user. CHEMKIN calculates the formation of molecules and excited states resulting from collisional processes and the absorption of solar and/or earthshine radiation. Although the code sets up the time-dependent differential rate equations, only the steady-state solution is currently used in obtaining the vibrational state populations.

The second component in the ambient population module is NEMESIS [Bernstein, 1988] (Non-Equilibrium Molecular Emission and Scattering Intensity Subroutine) which computes the enhancement of the atmospheric excited state layer populations due to layer radiative self-trapping and layer-layer radiative pumping. Some molecular bands, in particular the 4.3 μm CO_2 band, are optically opaque to emitted radiation. Photons emitted in these bands may be absorbed and emitted many times before either escaping the atmosphere or being collisionally quenched.

The overall approach for determining the enhanced excited-state level populations involves:

- determination of the steady-state layer source populations which includes excitation by external light sources, sun and earthshine, and molecular collisions, and de-excitation by radiative decay and collisional quenching (CHEMKIN);

- determination of the first-order layer-layer population enhancement using a Monte Carlo simulation of the initial source photon emissions and their subsequent absorption or escape (NEMESIS); and

- determination of the total enhanced populations using a recursive orders-of-enhancement approximation which is initialized by the Monte Carlo first-order results (NEMESIS).

The initial source populations include all excitation sources except the internal atmospheric radiative effects of layer self-trapping and layer-layer pumping. The key results from the Monte Carlo simulation are the first-order enhancements and the probabilities that a photon emitted from a layer "i" will create a new excited state in a layer "j". This simulation involves sampling over the initial emission position, emission direction, emission frequency, emission line strength, and length of travel. The contribution of each succeeding order-of-enhancement is determined recursively by

$$(P_k) = (P_{k-1})(W) \quad , \tag{28}$$

where (P_k) is the kth-order layer population enhancement matrix, and (W) is the layer-layer absorption probability matrix. Both (P_1) and (W) are determined by the first-order Monte Carlo calculation.

The end result of each NEMESIS calculation is the total excited-state population distribution for a pair of vibrational levels, where the lower level of each pair may itself be an excited level. A cycling procedure between CHEMKIN and NEMESIS is used to step up the vibrational energy ladder until the top of the ladder is reached.

3.2.4 The AURORA Population Routines

The AURORA routines calculate the change in the populations of CO_2, NO and NO^+ due to electron bombardment during an auroral storm. Default parameters for selecting auroras of different strength are contained in SAMM2; however, the user can easily define an aurora. The module performs a time dependent calculation to determine the auroral species number densities as a function of altitude. The Gear method [Kee *et al.*, 1980] for stiff differential equations is used to numerically integrate the chemical kinetic rate equations describing auroral chemical and energy transfer processes. This integration package is supplied as part of the Sandia CHEMKIN code [Kee *et al.*, 1980], and thus it has been extensively applied to and validated against many different types of scientific problems.

In addition to the normal SAMM2 inputs, the following inputs are required for the AURORA module:

- definition of the strength and duration of the aurora,
- specification of the chemical kinetics mechanism for the selected radiator, including primary and secondary electron processes.

The primary electron deposition model used in SAMM2 is based upon the work of Grun, Rees, and Strickland and has been discussed in some detail in the AARC manual [Winick *et al.*, 1987]. The SAMM2 routines describing the energy deposition have been derived from those used in AARC. The ion pair production rate is then obtained from the energy deposition rate by assuming that 35 eV are required to produce an ion pair.

The chemical reactions and energy transfer processes resulting from electron deposition in the atmosphere are also described in the AARC manual. Chemical kinetics mechanisms for NO, NO^+, and CO_2(4.3 μm) are supplied as part of the SAMM2 data base. The mechanisms include kinetic processes for ionization, electronic and vibrational excitation, recombination, chemical reactions, and formation of the secondary electron energy distribution. When the code exits from the auroral module, the aurorally enhanced populations are stored in an array for vibrationally excited species.

3.2.5 Determination of Population Fluctuations

The local temperature fluctuations induce fluctuations in the local vibrational state number densities. The influence of temperature and density enter into the chemical kinetic rate equations in a non-linear fashion. The collision rates are affected by temperature variations which alter rate constants and density variations which influence the number of collisions. The model predicts fluctuations in local vibrational state densities as a function of local temperature and density fluctuations. Temperature fluctuations cause two effects, a simple density expansion or compression which changes state populations induced by local heating or cooling respectively, and the adjustment of vibrational/rotational state populations due to chemical kinetic mechanism. In SAMM2, the rotational states are considered to be LTE, so rotational temperatures and fluctuations map exactly with kinetic temperature fluctuations. The variation of the vibrational state number densities are computed and stored in the "population file" for future use in determining the radiance statistics.

3.2.6 LOS Specification

The LOS specification routine breaks a LOS into small segments and determines the composition and properties of each segment. The segments are determined by the intersections of the LOS with the altitude layer boundaries, defined in the input atmospheric profiles. For each segment the region and solar zenith is found and the appropriate profiles, temperatures, pressures and molecular state number densities are determined. A more detailed description of how this is performed is provided Subsection 4.3.4.

3.2.7 The Radiation Transport Routines

SPCQBL computes the LOS spectral radiance using a finite-difference form of the radiative transfer equation [Bullitt *et al.*, 1985]. The LOS properties are specified in homogeneous segments along the LOS path from the observer to source. The Quasi-line-By-Line approach uses the Voigt lineshape to determine the segment transmittances and radiances. This approach enables the spectral radiance to be calculated at a maximum spectral resolution of 0.001 cm^{-1}. Since the radiation computation is explicitly based on the population difference of the upper and lower state, it is equally valid in both the NLTE and LTE regimes. Line strengths and locations are taken from a modified

line file generated from the 1996 AFGL HITRAN line atlas [Rothman *et al.*, 1998] and augmented with additional lines as outlined in Subsection 2.3. The major modification to the line parameter database was to decompose the energy of the lower state into vibrational and rotational energies. This enables the line strengths to be scaled separately for the rotational temperature and the NLTE vibrational population of the lower level.

There is a tradeoff between speed and accuracy when dividing the atmosphere into many homogeneous layers. The LOS radiance calculation depends linearly on the number of layers. Currently the atmospheres used by SAMM2 are layered by 1 km steps from 0 to 24 km, 2 km steps from 24 to 150 km and by 10 km steps from 150 to 300 km. For a single region limb calculation at a tangent height of 50 km with no relayering for atmospheric structure, 129 atmospheric layers are traversed by the LOS. Note that the atmospheric layering (maximum number of layers) currently used by SAMM2 can be changed by the user when the atmospheric profiles are generated by SAG-2. It should be pointed out that this is only necessary if the number of altitude layers is changed, not when different layer thicknesses are used.

3.2.8 The Radiance Statistics Routines

SAMM2 predicts a two dimensional radiance spatial covariance function from the vibrational state population fluctuations and temperature statistics along the user defined LOS. The covariance function is used by SAMM2 to determine radiance statistics for the LOS including the radiance variance, given by Equation (16), and horizontal and vertical correlation lengths/angles in the sensor image plane which is perpendicular to the LOS. The correlation lengths/angles are obtained by integration of the covariance function, Equation (15). The summary of the radiance statistics is printed to the general SAMM2 output file. Note that the radiance statistical parameters, variances and vertical correlation lengths, change with altitude and thus are non-stationary in the vertical direction. Since only the 1-D altitude profile is calculated, there is no change of the variance and horizontal correlation length with horizontal dimension. Thus, the statistics in the horizontal dimension is stationary. A future version of SAMM will calculate the horizontal dependence of these parameters. Meanwhile, multiple vertical scans may be calculated by SAMM2 (via single or batch mode) to create multiple output files of radiance statistics in the horizontal dimension. SIG

may then use the SAMM2 outputs to create a non-stationary scene in both the vertical and horizontal dimensions.

3.2.9 SAMM2 Output

The SAMM2 modules write data and informational statements to four user-readable ASCII data files. The files are the journal file which is called "SAMM2.LOG", the general output file (which contains the calculated radiance statistics), the spectral radiance file, and transmittance file. In addition, for each profile of each region there is a binary population file, whose name is specified by the user.

SAMM2.LOG contains various statements generated during a SAMM2 calculation. If SAMM2 recognizes a fatal problem, an error message is written to this file, and execution stops. A warning or caution is not fatal to SAMM2, but it may alert the user that only a partial calculation has been performed or that numerical difficulties have been encountered and fixed in some module. The user should get in the habit of looking at this file after every SAMM2 execution to insure that the full desired calculation was actually performed. During interactive input, the user has the option of specifying that caution and warning messages, which do not stop execution, be "suppressed," i.e., not printed to the file.

The output file contains a summary of the output from each module. In general, but not always, three levels of output are available for each SAMM2 module. The level of output is selected through the interactive menu and can be defined independently of other modules. The first level contains a minimum amount of information. For example, the minimum information on the model atmosphere is simply its name. The next level of output provides more detailed information such as the number densities of the atmospheric species as a function of altitude, or the vibrational temperatures from the chemical kinetics module. Finally, the highest level of output provides intermediate results from within modules. This level of information may be necessary for "debugging" a problem encountered in SAMM2, but it is usually too detailed for day-to-day execution.

The spectral and transmission files contain the spectral radiance and transmittance as a function of frequency. The resolution and frequency range are defined through the "SAMM2.INP" file. The

frequency unit is cm^{-1}, the radiance unit is W/sr/cm^2/cm^{-1}. This format is convenient for either plotting the calculated spectral radiance directly or for reducing these data further. For example, the user may wish to apply a specific filter function to the spectral radiance or to convert to a set of units other than those used in SAMM2. These manipulations can be performed using the "DEGRAD" program (see Subsection 7.4).

The population file saves the excited state populations and other necessary information so multiple SAMM2 calculations can be performed without re-calculating the populations each time. There are two types of population files, ambient and auroral. The two types of population files have different formats, so they can be used only with the proper environment type. Populations calculated from a model atmosphere will change only when either a new model atmosphere is used, day and night conditions change, a new solar zenith angle is defined, or auroral parameters are changed. By saving and re-using these population files, a user can build up a library of population files for simulations of interest, thus saving considerable time. Population files can be reused for multiple LOS traversing the same atmospheric regions, and for different spectral intervals. The interactive input module will warn the user if an attempt is made to modify parameters which effect populations, when an old population file is in use. These warnings become errors if the code is run in batch mode. The errors are detected prior to computation. Messages describing the errors are written in the SAMM2.LOG file.

4. RUNNING SAMM2

4.1 Overview

This section serves as a reference for the user who wants to get SAMM2 running without making modifications to the chemical kinetics mechanisms supplied with the code. The required files and auxiliary programs are discussed, allowing preparation of the first run. The menu system used by the INPUT module to communicate with the user is outlined in some detail. This is followed by discussions of some of the more important parameters entered through the menus. The user should read Section 3 through the end of Subsection 3.1 before reading this section. If modifications to the kinetics files are required, the user should first read Sections 6 and 7 below.

Prior to the first SAMM2calculation, the binary "lines" files must be created. Default kinetics linking files are provided with the code as ASCII files. As discussed below, these "linking" files and their associated states and bands files need not be in the same directory as the executable version of SAMM2; rather, they should be placed in a separate "kinetics" directory for convenience. The spectral lines files are supplied in ASCII form as SAMM96.ASC, LTETAILS.ASC, and VOIGTPROFILE.ASC. Conversion to the binary forms used by SAMM2 is carried out by short programs (binary_lines.f, binary_tails.f, and binary_voigt.f) which the user must compile and run. After running these three programs, three *.bin files are created, which must be located in the LINES directory.

Once the user has prepared the above files, SAMM2 can be executed. It can be run in either an interactive or batch/background mode. The interactive mode is useful in setting up new calculational scenarios, since it walks the user through the necessary input variables. For more experienced users, SAMM2 can be executed by circumventing the input module and directly entering changes to the SAMM2.INP file with an editor.

After a successful SAMM2calculation there will be four or more new output files. These files are:

- Journal file   (described in Subsection 5.1),
- General output file   (described in Subsection 5.2),

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- Population files   (described in Subsections 5.3 and 5.7),
- Spectral radiance file   (described in Subsection 5.4),
- Band radiance file   (described in Subsection 5.5),
- Transmittance file   (described in Subsection 5.6), and
- Radiance structure statistics files   (described in Subsection 5.7).

The journal file, called SAMM2.LOG, should be empty if the calculation was performed without errors, warnings, or cautions. The user should always check this file to insure the calculation was performed correctly. The general output file summarizes the calculation. The transmittance file contains two columns giving the LOS transmission as a function of frequency (cm^{-1}). The spectral radiance file contains the spectral radiance ($W/sr/cm^2/cm^{-1}$) as a function of frequency (cm^{-1}). The population file contains the excited-state population information so that subsequent calculations can skip the population modules and go directly to the LOS specification and spectral radiance modules. To repeat for added emphasis, populations depend only on the molecular species, model atmosphere, auroral parameters, day/night conditions, and/or solar zenith angle; therefore, the same populations can be used for many different LOS's and bandpass configurations. This can save considerable computer time, and the user should develop a library of populations for often-used scenarios.

4.2 The Interactive Input Module

The SAMM input module uses a menu-query system to walk the user through the required inputs. In general, typing a 0 will take the user up a level in the menu system, while typing a number greater than 0 allows the user to input new information or enter a submenu. When a submenu is entered, current values of the input variables are displayed. This allows the user to scan the current values and decide if anything needs to be changed. The precise sequence of menus depends on choices made by the user and cannot be presented in any compact listing. Here, only the major menus will be discussed.

At the start of an interactive run, the top-level menu appears:

```
SHARC AND MODTRAN MERGED, SAMM2

 REVIEW OR MODIFY INPUT PARAMETERS

 1) TITLE FOR CALCULATION
 2) REGION DEFINITION (TEMPERATURE STATISTICS INPUT)
 3) LOS GEOMETRY (LOS RADIANCE STATISTICS/SCENE INPUT)
 4) SPECTRAL INTERVAL, RESOLUTION AND SPECIES
 5) OUTPUT DATA
 6) STANDARD SET-UP FOR FILE NAMES

 7) INSTALLATION SETUP

 8) UPDATE DEFAULT FILE AND EXIT FOR BATCH EXECUTION
 9) UPDATE DEFAULT FILE AND EXIT
 10) EXIT WITH NO UPDATE OF DEFAULT FILE

 ENTER # OF ITEM TO BE CHANGED OR
 999 TO CONTINUE SAMM EXECUTION
```

The latter entries govern subsequent modes of execution of SAMM. An "8" exits SAMM, saving any changes that may have been made to the SAMM.INP file; a parameter is set so that the next time SAMM is run it will be in the "batch" mode, skipping the interactive session. Exiting with a "9" saves the changes but prepares for an interactive run next time. If the user wants to start over with the original input file, a "10" exits without saving any changes, and SAMM will next start in interactive mode.

The installation setup menu, item 7, which allows the user to specify directory paths for the data files, should be executed first. Also, file name patterns are set here, which eases the task of specifying file names in other parts of the menu tree. A sample menu 7 appears below as a second-level menu display. All directory and file name examples shown in this manual conform to UNIX name conventions. The directory and file names entered by the user are concatenated and stored in string variables used in the "OPEN" statements for those files. This scheme will work for non-UNIX systems if the user employs file and directory naming conventions appropriate to those systems.

```
7) REVIEW OR MODIFY SET-UP STRUCTURES

 1. DIRECTORY PATH FOR THE CHEMICAL KINETICS FILES
         kindir/
 2. PREFIXES AND SUFFIXES FOR LINKING FILES
       AMBIENT (FORMULA).LNK      AURORAL A(FORMULA).LNK
 3. PREFIXES AND SUFFIXES FOR STATES  FILES
       AMBIENT (FORMULA).STA      AURORAL A(FORMULA).STA
 4. PREFIXES AND SUFFIXES FOR BANDS  FILES
         AMBIENT (FORMULA).BND
 5. CASE SELECTION FOR KINETICS FILES   UPPER
 6. DIRECTORY PATH FOR THE PROFILES
         atmdir/
 7. CASE SELECTION FOR PROFILES         UPPER
 8. DIRECTORY PATH FOR THE POPULATIONS
         popdir/
 9. CASE SELECTION POPULATION FILES    UPPER
10. SUPPRESSION OF RUN TIME WARNINGS  NOSUPPRESSION
11. DIRECTORY PATH FOR THE LINES FILE
         lines/
12. LINES FILE NAME                        SAMM96.BIN
13. EXTENDED LTE LINE TAILS FILE NAME      LTETAILS.BIN
14. VOIGT LINE SHAPE PARAMETERS FILE NAME VOIGTPROFILE.BIN

ENTER  # OF ITEM TO BE CHANGED OR
         0 TO CONTINUE
```

The user may specify different paths to various file groups. Menu item 1, specifies the path name to the kinetics (states, bands, binary linking and lower altitude continuum transmittance) files. The file naming convention is fixed as (molecular formula).CNT. For example, for OH, the continuum transmittance file name is OH.CNT. In menu item 6 the path name to the atmospheric profiles, in menu item 8 the path name to the population files, and in menu item 11 the path name to the lines file can be specified.

The full file names will be formed by appending the species file name to the directory name. Thus, the directory name for UNIX systems must always end in a "/", so that the full path name will be correct. For DOS systems the directory name must end in a back slash "\". To maintain compatibility with all operating systems, SAMM does not supply the missing delimiter "/" or "\". The users must supply the appropriate delimiter when entering the directory name. If new population files are being generated, they will be placed in the directory specified. Items 2 through 5 and 7

specify the pattern a species or atmosphere file name will follow. When Item 2 is chosen, for example, the user will be prompted for prefixes and suffixes which will be attached to the species name. Each species name is simply its chemical formula with the exception of ions where a "P" is used for plus and an "M" for minus charge. For example for NO^+, the species' name in file names is NOP. This conforms with MS-DOS restrictions on use of special characters in file names.

If a new species is requested while the user is defining a region, these prefixes and suffixes will automatically be attached to create the proper file name. Null strings are acceptable, and case is determined by Items 5 and 7. Note that a change here will only affect newly chosen file names; names previously determined will not be changed unless the user goes to Item 2 of the top-level menu and makes the change. The only specific file name determined here is that of the lines file, which contains information for all species.

The first item 1, in the top-level menu permits setting the title of the calculation, which appears in the output file. The second item defines the atmospheric regions and leads to the most extensive set of sub-menus. The second-level menu of this set lists by number the regions already defined and permits definition of new ones. An example appears below.

```
2) REVIEW OR MODIFY REGION DEFINITIONS

 CURRENTLY THERE ARE  1 REGIONS: 1 EXTENDED AND  0 LOCAL

 1. EXTENDED REGION IS AMBIENT WITH  7 PROFILE(S)

 ENTER # OF REGION TO REVIEW OR MODIFY OR
        -# TO DELETE REGION OR
        2 TO ADD REGION OR
        0 TO CONTINUE
```

Only one region has been defined thus far; this menu only tells the user that Region 1 uses 7 atmospheric profiles. Typing "1" selects Region 1 for inspection:

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```
REGION DEFINITION DATA FOR REGION # 1

  1- REGION IS AMBIENT WITH   7 PROFILE(S)
  2- SOLAR ZENITH ANGLES   LOWER ATMOSPHERE AEROSOL NUMBERS
  3- MODEL ATMOSPHERE FILE NAMES
     FOR  SOLAR ZENITH  =   100.88   T4Z101.ATM
     FOR  SOLAR ZENITH  =   101.68   T4Z102.ATM
     FOR  SOLAR ZENITH  =    98.65   T4Z99.ATM
     FOR  SOLAR ZENITH  =    97.01   T4Z97.ATM
     FOR  SOLAR ZENITH  =    95.27   T4Z95.ATM
     FOR  SOLAR ZENITH  =    93.06   T4Z93.ATM
     FOR  SOLAR ZENITH  =    90.85   T4Z91.ATM
  4- EXTRA-TERRESTRIAL SOURCE – SUN
  5- GROUND DEFINITION
  6- CURRENT POPULATION FILE NAMES
  7- MONTE CARLO RADIATION TRANSPORT INPUTS
  8- TEMPERATURE STATISTICS INPUTS
  9- MOLECULAR RADIATORS FOR POPULATION CALCULATION
       AMBIENT: O3
 10- NO MULTIPLE SCATTERING CALCULATION

ENTER # OF ITEM TO CHANGE OR
        0 TO CONTINUE
```

In this third-level menu, Item 1 allows setting the type of the region (ambient or auroral; Region 1 must always be ambient) and the number of atmospheric profiles. Each profile must have an associated file name for its defining atmosphere file (the file name also appears in the atmosphere file), a solar zenith angle for the solar pumping calculation, and a lower-atmosphere continuum (aerosol) index. The aerosol index influences the absorbing effect of the lower atmosphere on sunlight when the sun is below the horizontal, as discussed more fully in Subsection 6.4. The zenith angles and aerosol indices are set under Item 2. The association of angles with file names is made under Item 3; the current angles and file names are shown in the example above. The number of files and angles can also be reduced; choosing "1" and then entering a number less than 7 would truncate the list of atmospheric profile file names appearing under Item 3. In this example, the file names incorporate the values of their respective solar zenith angles; this correspondence is not required but is recommended.

Item 4 in the "REGION DEFINITION" menu allows the user to specify the extra-terrestrial source and irradiance for the molecular solar/lunar pumping and the multiple scattering of solar/lunar irradiance. Note that Item 4 only appears for Region #1 (ambient). An unscaled solar source is specified in the following menu:

```
EXTRA-TERRESTRIAL SOURCE

  1 - SOLAR IRRADIANCE INPUT FILE : NEWKUR.DAT
        WITH NO SOLAR IRRADIANCE SCALE FACTOR
  2 - SELECT MOON

ENTER # OF ITEM TO BE SELECTED OR
        0 TO CONTINUE
```

This fourth-level menu allows the user to change the solar irradiance model or to select the moon as the extra-terrestrial source. Note that the user must enforce the consistency between the choice of the extra-terrestrial source and the specification of the solar zenith angle in the REGION DEFINITION (third-level) menu. Selecting a "1" presents the user with the option to change the solar irradiance input file or enter a solar irradiance scaling factor.

```
MODIFY SOLAR IRRADIANCE

  1 - SOLAR IRRADIANCE INPUT FILE : NEWKUR.DAT
  2 - NO SOLAR IRRADIANCE SCALE FACTOR

ENTER # OF ITEM TO BE CHANGED OR
        0 TO CONTINUE
```

By selecting "1" in this fifth-level menu, the user can choose one of the four provided solar irradiance data bases or enter a file name for a user-defined data base, which must be located in the directory specified by Item 6 (DIRECTORY PATH FOR THE PROFILES) in the second-level menu REVIEW OR MODIFY SET-UP STRUCTURES described previously.

```
SELECT SOLAR IRRADIANCE DATA BASE

   1 - CORRECTED KURUCZ DATA BASE
   2 - CHANCE DATA BASE
   3 - CEBULA PLUS CHANCE DATA BASE
   4 - THUILLIER PLUS DATA BASE CORRECTED KURUCZ
   5 - USER-DEFINED SOLAR IRRADIANCE DATA BASE

ENTER # OF ITEM TO BE CHANGED OR
       0 TO CONTINUE
```

Scaling the solar irradiance is accomplished by entering "2" in the MODIFY SOLAR IRRADIANCE menu, resulting in the following menu:

```
SELECT SOLAR IRRADIANCE SCALE FACTOR

   1 - SCALE THE SOLAR IRRADIANCE
   2 - DO NOT SCALE THE SOLAR IRRADIANCE
   3 - RENORMALIZE THE SOLAR CONSTANT

ENTER # OF ITEM TO BE CHANGED OR
       0 TO CONTINUE
```

The user can choose to scale the solar irradiance (menu Item 1) by a scale factor ($0.9 <$ scale factor < 1.1) or to not scale the solar irradiance (menu Item 2). Alternatively, the user can use menu item 3 to renormalize the solar irradiance by specifying the solar constant (in W/m^2), which is the spectrally-integrated value of the solar irradiance. An additional scaling of the solar irradiance value to account for earth-to-sun distance is also applied based on the day of the year.

To select the moon as the (reflected solar) extra-terrestrial source, the user enters a "2" in the fourth-level EXTRA-TERRESTRIAL SOURCE menu. The resultant menu requires the user to input the moon phase angle:

```
INPUT PHASE ANGLE OF THE MOON (DEGREES)

   ENTER 0 FOR FULL MOON,
         90 FOR HALF MOON,
         180 FOR NO MOON
```

For example, if the user enters 95 ° for the phase of the moon, the following menu is presented:

```
EXTRA-TERRESTRIAL SOURCE

  1 - MOON PHASE ANGLE (DEGREES) : 95.
  2 - SOLAR IRRADIANCE INPUT FILE : NEWKUR.DAT
        WITH NO SOLAR IRRADIANCE SCALE FACTOR
  3 - SELECT SUN

ENTER # OF ITEM TO BE SELECTED OR
        0 TO CONTINUE
```

The user can also change and/or scale the lunar (solar reflected) irradiance source function (menu item 2) as described above.

The user can characterize the reflective/emissive properties of the ground by selecting Item 5 in the REGION DEFINITION menu, which displays the current values of the terminal temperature of the LOS (in this example, the temperature of the first atmospheric layer is used as the terminal (boundary) temperature of the LOS), ground altitude with respect to sea level (0 km), and the optical properties for the surface (a spectrally independent value of the surface albedo of 0.0). Note that Item 5 only appears for Region #1 (ambient).

```
GROUND DEFINITION

  1 - BOUNDARY TEMPERATURE FROM FIRST ATMOSPHERIC LAYER
  2 - GROUND ALTITUDE WRT SEA LEVEL (KM) : 0.E+0
  3 - SPECTRALLY INDEPENDENT SURFACE ALBEDO : 0.E+0

ENTER # OF ITEM TO BE CHANGED OR
        0 TO CONTINUE
```

The temperature for the terminal point (H2) of the LOS can be modified by selecting Item 1 in this fourth level GROUND DEFINITION menu, presenting the user with the menu:

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```
MODIFY BOUNDARY TEMPERATURE

  1 - INPUT BOUNDARY TEMPERATURE
  2 - USE TEMPERATURE OF FIRST ATMOSPHERIC LAYER

ENTER # OF ITEM TO BE CHANGED OR
       0 TO CONTINUE
```

The user can choose to input the temperature for the terminal point of the LOS by selecting "1" and then entering a value of the temperature in Kelvin, say 300. The user is then returned to the GROUND DEFINITION menu. The emission contribution to the LOS radiance is computed using this value of the temperature. Note that if the user has specified one of the multiple LOS options in the geometry menu, this temperature is used as the terminal temperature for each LOS. If no emission is desired, a value of 0 K should be entered for the temperature.

Item 2 in the GROUND DEFINITION menu permits the definition of the altitude of the surface relative to sea level. The entered value (in km) may be negative but may not exceed 6 km. The baseline 0 to 6 km aerosol profiles are compressed (or stretched) based on this input. The default value is the altitude of the first atmospheric level.

```
MODIFY GROUND ALTITUDE

  INPUT GROUND ALTITUDE RELATIVE TO SEA LEVEL (KM)
```

Entering a value for the ground altitude, i.e., 5.0, returns the user to the GROUND DEFINITION menu.

```
GROUND DEFINITION

  1 - BOUNDARY TEMPERATURE (K) : 300.
  2 - GROUND ALTITUDE WRT SEA LEVEL (KM) : 5.E+0
  3 - SPECTRALLY INDEPENDENT SURFACE ALBEDO : 0.E+0

ENTER # OF ITEM TO BE CHANGED OR
       0 TO CONTINUE
```

The optical properties of the surface are currently defined by a spectrally independent surface albedo of 0. In addition to the spectrally independent Lambertian model, the user has several options available to select a spectral surface reflectance model. Entering "3" in the "GROUND DEFINITION" menu gives the user the choice of a spectral BRDF Model, a spectral Lambertian Model, or to change the (currently selected) value of the spectrally independent surface albedo:

```
SURFACE REFLECTANCE MODEL

    1 - SELECT SPECTRAL BRDF MODEL
    2 - SELECT SPECTRAL LAMBERTIAN MODEL
    3 - MODIFY SPECTRALLY INDEPENDENT ALBEDO : 0.E+0

ENTER # OF ITEM TO BE CHANGED OR
        0 TO CONTINUE
```

To change the value of the spectrally independent surface albedo, enter 3, followed by the value (between 0 and 1) of the surface albedo.

If the user wishes to select a spectral BRDF or Lambertian surface reflectance model, the value of 1 or 2 is entered in the SURFACE REFLECTANCE MODEL menu, respectively. For example, to select a spectral BRDF model, enter "1", resulting in the following menu for the BRDF model and parameters:

```
SELECT SPECTRAL BRDF MODEL AND PARAMETERS

    1 - SPECTRAL BRDF MODEL
    2 - BRDF MODEL PARAMETERS INPUT FILE NAME

ENTER # OF ITEM TO BE SELECTED OR
        0 TO CONTINUE
```

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The user can then select one of seven available BRDF models (see Section 6.8.2) and/or specify the name of the file containing the associated BRDF parameters. By entering "1", the submenu containing the BRDF models is presented as shown below:

```
SELECT ONE OF THE AVAILABLE BRDF MODELS

   2 - WALTHALL
  51 - WALTHALL_A
  11 - SINE-WALTHALL
  52 - SINE-WALTHALL_A
   4 - HAPKE
   5 - RAHMAN
   6 - ROUJEAN
  10 - PINTY-VERSTRAETE
  12 - ROSS-LI

ENTER # OF ITEM TO BE SELECTED OR
       0 TO CONTINUE
```

The file name for the spectral BRDF parameters is specified by selecting Item 2 and either accepting the default file name or entering the file-specified file name. For example, if the user selects Item "2" from the available BRDF models (corresponding to the Walthall model), there is a prompt to use the default BRDF file name, WALTHALL.DAT, or enter a user-specified name:

```
DEFAULT SPECTRAL BRDF FILE NAME IS WALTHALL.DAT

ENTER NEW SPECTRAL BRDF FILE NAME OR
  0 TO CONTINUE
```

The user can then accept the default BRDF file name by entering "0" or enter a new BRDF file name. The BRDF parameters files must be located in the directory specified by Item 6 (DIRECTORY PATH FOR THE PROFILES) in the second-level menu REVIEW OR MODIFY SET-UP STRUCTURES described previously. It is important to note that the user must be prepared to supply the appropriate model parameters for the selected BRDF model, as only representative parameters are provided for illustrative purposes.

To select a spectral Lambertian surface reflectance model, enter "2" in the SURFACE REFLECTANCE MODEL menu which then displays the list of materials available from the MODTRAN4 database [Berk et al., 19]

```
SELECT SPECTRAL SURFACE ALBEDO FOR ONE OF THE FOLLOWING MATERIALS

   1 - FRESH SNOW
   2 - FOREST
   3 - FARM
   4 - DESERT
   5 - OCEAN
   6 - CLOUD DECK
   7 - OLD GRASS
   8 - DECAYED GRASS
   9 - MAPLE LEAF
  10 - BURNT GRASS
  21 - CONSTANT 5% REFLECTIVITY
  22 - CONSTANT 50% REFLECTIVITY
  31 - CCM3 SEA ICE
  99 - USER-DEFINED MATERIAL

ENTER # OF ITEM TO BE SELECTED OR
        0 TO CONTINUE
```

The user can choose one of the supplied materials or provide a user-defined reflectance data set by selecting "99". After selecting the desired material, the option to accept the default file (SPEC_ALB.DAT) containing the reflectance data base or input a user-defined name. The spectral albedo parameters files must be located in the directory specified by Item 6 (DIRECTORY PATH FOR THE PROFILES) in the second-level menu REVIEW OR MODIFY SET-UP STRUCTURES described previously. If the user selects item 2 (FOREST) in the above menu and selects the default spectral albedo file, the following GROUND DEFINITION menu appears:

```
GROUND DEFINITION

   1 - BOUNDARY TEMPERATURE (K) : 300.
   2 - GROUND ALTITUDE WRT SEA LEVEL (KM) : 5.E+0
   3 - SPECTRAL LAMBERTIAN SURFACE : FOREST
       USING SPECTRAL ALBEDOS FROM INPUT FILE : SPEC_ALB.DAT
```

```
ENTER # OF ITEM TO BE CHANGED OR
        0 TO CONTINUE
```

Item 6 permits the user to specify the names of the binary population files which store the results of the CHEMKIN/NEMESIS calculation. One population file is created for each atmospheric profile. The user can determine that preexisting population files be used for any of the profiles; in this case SAMM omits the CHEMKIN/NEMESIS step, saving much time. If new population data are to be calculated but not saved, scratch file names can be given for population files later discarded. A sample menu (a fourth-level menu) brought up by Item 6 follows:

```
POPULATION FILE NAME(S) AND STATUS

PROFILE # 1
NEW AMBIENT                     T4Z102.POP
PROFILE # 2
NEW AMBIENT                     T4Z101.POP
PROFILE # 3
NEW AMBIENT                     T4Z99.POP
PROFILE # 4
NEW AMBIENT                     T4Z97.POP
PROFILE # 5
NEW AMBIENT                     T4Z95.POP
PROFILE # 6
NEW AMBIENT                     T4Z93.POP
PROFILE # 7
NEW AMBIENT                     T4Z91.POP

ENTER PROFILE # OF THE POPULATION FILE(S) TO BE DEFINED OR
        0 TO CONTINUE
```

Initially an auroral region would have one OLD ambient population file and a NEW auroral file for each profile in the region.

Item 7 in the region definition menu permits setting several parameters for the NEMESIS Monte Carlo calculation. The number of trial photons and the maximum order of scattering determine the statistical error of the calculation. The user also specifies in this menu whether the SAMM calculation will use earthshine or not. See Subsection 4.3.1.

Item 8 allows the user to specify the temperature statistics inputs for atmospheric structure calculations. The dialog boxes encountered under Item 8 are discussed later in this section. The first menu (fourth-level) under Item 8 shows the following:

```
SUMMARY OF STRUCTURE CALCULATION

 1. STRUCTURE CALCULATION ENABLED
 2. NON-STATIONARY ATMOSPHERE
    USING TEMPERATURE STATISTICS FILE : STATS_MSX.DAT
 3. SCALING FACTORS
    STANDARD DEVIATION SCALED BY  1.0
    VERTICAL CORRELATION LENGTH SCALED BY  1.0
    HORIZONTAL CORRELATION LENGTH SCALED BY  1.0
 4. SPECTRAL INDICIES FOR TEMPERATURE PSD
    VERTICAL TEMPERATURE SPECTRAL INDEX   : -3.0
    HORIZONTAL TEMPERATURE SPECTRAL INDEX : -1.67

ENTER # OF ITEM TO BE CHANGED OR
      0 TO CONTINUE
```

If the user select Item 1 in this menu a submenu is displayed which allows the user to turn on and off the SAMM structure option. As structure in the region is currently enabled, the following submenu (fifth-level) is shown:

```
RADIANCE STRUCTURE CALCULATION

ENTER 1 FOR NO STRUCTURE IN REGION OR
      0 TO CONTINUE
```

Other important temperature structure information available in this section of the menus includes the definition of an external file containing the temperature statistics as a function of altitude, scaling factors for the temperature statistics and the assumed spectral indices for the temperature PSD, where the spectral index is defined as the slope of the PSD in LOG-LOG space. This last input option is shown below.

```
SPECTRAL INDICES FOR TEMPERATURE PSD
```

```
1) VERTICAL SPECTRAL INDEX   : -3.0
2) HORIZONTAL SPECTRAL INDEX : -1.67

ENTER # OF ITEM TO BE CHANGED OR
        0 TO CONTINUE
```

The radiators for the CHEMKIN/NEMESIS calculation are identified in Item 9 of the region definition menu. Choosing this item results in a display of radiators currently selected and the opportunity to modify or review them. In the following example, ozone is the only radiator selected.

```
AMBIENT RADIATORS ARE:
        O3   ISOTOPE 16O 16O 16O

ENTER SPECIES MOLECULAR FORMULA TO ADD OR REVIEW DATA
  - MOLECULAR FORMULA TO REMOVE SPECIES
  0 TO CONTINUE
```

If the user enters the molecular formula, "O3", the names of the present data files for that species are displayed, and the opportunity to modify them is presented:

```
        REVIEW OF O3   INPUT DATA
        AMBIENT DATA
   #    ISOTOPE      LINKING      STATES      BANDS
   1    16O 16O 16O        O3.LLL      O3.SSS      O3.BBB

ENTER # OF ITEM TO CHANGE OR
        0 TO CONTINUE
```

Typing "1" would allow the user to modify the file names. Had the user instead entered a new formula, the program would have confirmed the species to be entered, and file names would have been constructed according to the patterns discussed above. These would have been displayed to the user in the manner shown above. The user would again have the opportunity to modify the radiators. Had the user named a species for which more than one isotope is supported, the program would have detoured through a series of menus requesting specification of which isotopes were wanted before reaching the file name review menu. In this case, each isotope would have its own line in that

menu, allowing independent review of each set of file names. The review step, if chosen, also displays the relative abundance of each isotope, the fraction of all molecules of a species which have that particular isotopic composition. For molecules where the separate isotopes are not distinguished in this release, the abundance equals 1.00. For the first isotope of CO_2, in contrast, the abundance equals 0.984.

Note that the O_3 file names above do not correspond to the pattern set down previously in the installation setup menu, Item 7 of the top-level menu. That pattern would have led to the names O3.CKL, O3.STA, and O3.BND. The actual file names differ either because they were entered under a different, earlier set of name patterns, or because they were created by directly editing the input file. This difference emphasizes the fact that setting a name pattern in the setup menu does not insure that these names will be used. Precedence is given to edited names; the setup names are invoked when the user adds species. The user should always check the file names. In the present menu, the switch to the *.CKL, *.STA, and *.BND patterns is most easily accomplished by removing O_3 as an included species (typing "-O3") and then adding it again (typing "O3"). The addition process will create file names with the pattern specified in the setup. If, on the other hand, O_3 is being added and the *.LLL, *.SSS, *.BBB patterns are wanted despite the setup, the user can change individual file names in the review step. The linking, states and bands files are stored along with the low altitude transmittance (continuum) files in the same directory specified in the setup. Regardless of the naming of the particular linking or states files for O_3 the O3.CNT file will be used.

In the current example, if the user backs up two levels in the menu tree (by entering "0" twice), the second-level menu will again be displayed:

```
2) REVIEW OR MODIFY REGION DEFINITIONS

 CURRENTLY THERE ARE  1 REGIONS: 1 EXTENDED AND  0 LOCAL

 1. EXTENDED REGION IS AMBIENT WITH  7 PROFILE(S)

 ENTER # OF REGION TO REVIEW OR MODIFY OR
       -# TO DELETE REGION OR
       2 TO ADD REGION OR
       0 TO CONTINUE
```

Entering "2" will bring up the region definition menu for the entirely undefined Region 2:

```
NEW REGION PARAMETERS FOR REGION # 2

  1- REGION ENVIRONMENT AND STRUCTURE
  2- SOLAR ZENITH ANGLE   LOWER ATMOSPHERE AEROSOL NUMBER
  3- MODEL ATMOSPHERE FILE NAME
  4- INPUT NEW POPULATION FILE NAMES
  5- MONTE CARLO RADIATION TRANSPORT INPUTS
  6- TEMPERATURE STATISTICS INPUTS
  7- MOLECULAR RADIATORS FOR POPULATION CALCULATION
  8- AURORAL MODEL PARAMETERS
  9- REGION BOUNDARIES

ENTER # OF ITEM TO INPUT DATA OR
        0 TO CONTINUE
```

The user would then proceed through the options much as before, entering the various parameters. Note that all regions after the first one are local. They may be auroral, so Items 8 and 9 for setting auroral and boundary parameters appear for the first time. The auroral parameters are discussed in Subsection 4.3.2.

SAMM2 allows the user to include the aerosol/cloud emissive and scattered radiance contributions to the atmospheric attenuation and path radiance. This multiple scattering capability can only be employed in the extended atmospheric region, i.e., one cannot include cloud/aerosol scattering in local regions. The MODTRAN4 multiple scattering (MS) models and cloud/aerosol databases [Berk *et al.*, 1999] are accessed by entering "10" in the REGION DEFINITION menu, displaying the following MULTIPLE SCATTERING choice:

```
NO MULTIPLE SCATTERING CALCULATION

ENTER 1 FOR MULTIPLE SCATTERING CALCULATION OR
        0 TO CONTINUE
```

Entering "1" to select a MS calculation loads the default multiple scattering menu, which allows the user to select and/or modify the MS algorithm and define the cloud/aerosol properties:

```
SUMMARY OF MULTIPLE SCATTERING CALCULATION

  1. MULTIPLE SCATTERING ALGORITHM
     8-STREAM DISORT MODEL WITH NO AZIMUTH DEPENDENCE
  2. AEROSOL DESCRIPTION
     RURAL EXTINCTION, VIS=23 KM
     SPRING-SUMMER PROFILE
     BACKGROUND STRATOSPHERIC PROFILE AND
     NO ARMY VERTICAL STRUCTURE ALGORITHM FOR BOUNDARY LAYER
     DEFAULT VISIBILITY ASSUMED
     NO SHIFTING OR SCALING OF AEROSOLS
     DEFAULT AEROSOL SCATTERING PHASE FUNCTION FROM MIE THEORY
  3. CLOUD DESCRIPTION
     CUMULUS CLOUD LAYER; BASE=0.66 KM, TOP=3.0
     NO RAIN
     DEFAULT CLOUD MODEL PARAMETERS

ENTER # OF ITEM TO BE CHANGED OR
        0 TO CONTINUE
```

To change the MS algorithm, enter "1", which then displays the menu:

```
MULTIPLE SCATTERING ALGORITHM

   8-STREAM DISORT MODEL WITH NO AZIMUTH DEPENDENCE

ENTER 1 TO MODIFY ALGORITHM OR
        0 TO CONTINUE
```

To modify the MS algorithm or change the DISORT parameters to be used, enter "1" to display the menu:

```
SELECT MULTIPLE SCATTERING ALGORITHM

   1 - 2-STREAM ISAAC MODEL
   2 - 2-STREAM DISORT MODEL
   3 - 4-STREAM DISORT MODEL
   4 - 8-STREAM DISORT MODEL
   5 - 16-STREAM DISORT MODEL

ENTER # OF ITEM TO BE SELECTED OR
        0 TO CONTINUE
```

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This menu allows the user to select either the (fast/less accurate) ISAACS 2-stream model or the number of streams to be used by the DISORT. Using a high number of streams generally improves accuracy but slows computation. The 8-stream model is recommended for most application, although more streams are desirable if modeling highly forward peaked scattering phase functions. DISORT has been optimized for 4-, 8- and 16-streams only. To select the 4-stream DISORT model, enter "3", which then displays the menu,

```
SELECT AZIMUTHAL DEPENDENCE FOR DISORT MODEL

ENTER 0 FOR NO AZIMUTHAL DEPENDENCE OR
      1 FOR AZIMUTHAL DEPENDENCE
```

allowing the user to decide whether or not to include the azimuthal dependence in the line-of-sight multiple scattering solar calculation. Since this option increases computation time, no azimuthal dependence should be selected if only vertical fluxes are needed, if solar or viewing zenith angle is near vertical, or if solar multiple scattering is a small radiance component (e.g. for LWIR calculations). By entering "1", the MS calculation is summarized in the following menu:

```
SUMMARY OF MULTIPLE SCATTERING CALCULATION

 1. MULTIPLE SCATTERING ALGORITHM
    4-STREAM DISORT MODEL WITH AZIMUTH DEPENDENCE
 2. AEROSOL DESCRIPTION
    RURAL EXTINCTION, VIS=23 KM
    SPRING-SUMMER PROFILE
    BACKGROUND STRATOSPHERIC PROFILE AND
    NO ARMY VERTICAL STRUCTURE ALGORITHM FOR BOUNDARY LAYER
    DEFAULT VISIBILITY ASSUMED
    NO SHIFTING OR SCALING OF AEROSOLS
    DEFAULT AEROSOL SCATTERING PHASE FUNCTION FROM MIE THEORY
 3. CLOUD DESCRIPTION
    CUMULUS CLOUD LAYER; BASE=0.66 KM, TOP=3.0
    NO RAIN
    DEFAULT CLOUD MODEL PARAMETERS

ENTER # OF ITEM TO BE CHANGED OR
        0 TO CONTINUE
```

To remove aerosols or modify the aerosol description, the user now enters "2", which displays the menu

```
AEROSOL MULTIPLE SCATTERING CALCULATION

  1 FOR NO AEROSOLS
  2 MODIFY AEROSOLS

ENTER # OF ITEM TO BE SELECTED OR
        0 TO CONTINUE
```

Entering "2" displays the aerosol properties listed in the following menu:

```
MODIFY AEROSOL DESCRIPTION

  1 - RURAL EXTINCTION, VIS=23 KM
  2 - SPRING-SUMMER PROFILE
  3 - BACKGROUND STRATOSPHERIC PROFILE AND EXTINCTION
  4 - NO ARMY VERTICAL STRUCTURE ALGORITHM FOR BOUNDARY LAYER
  5 - DEFAULT VISIBILITY ASSUMED
  6 - DEFAULT AEROSOL SCATTERING PHASE FUNCTION FROM MIE THEORY

ENTER # OF ITEM TO BE CHANGED OR
        0 TO CONTINUE
```

Currently the altitude profile and extinction coefficients are defined by a rural aerosol (with default visibility (VIS) of 23 km) for the boundary layer (0 to 2 km) with a spring-summer profile for the tropospheric (2 to 10 km) and stratospheric (10 to 30 km) aerosols, and a background stratospheric aerosol model for the stratosphere (10 to 30 km) and mesosphere (30 to 100 km). The user can select a different boundary layer aerosol and/or default visibility by entering "1", displaying the following BOUNDARY LAYER AEROSOL EXTINCTION menu:

```
SELECT BOUNDARY LAYER AEROSOL EXTINCTION

  1 - RURAL EXTINCTION, VIS=23 KM
  2 - RURAL EXTINCTION, VIS=5 KM
  3 - NAVY MARITIME EXTINCTION, VIS BASED ON WIND SPEED/HUMIDITY
  4 - NAVY MARITIME EXTINCTION, VIS=23 KM
  5 - URBAN EXTINCTION, VIS=5 KM
```

```
6 - TROPOSPHERIC EXTINCTION, VIS=50 KM
7 - USER-DEFINED EXTINCTION
8 - FOG1 EXTINCTION(ADVECTIVE) VIS=0.2 KM
9 - FOG1 EXTINCTION(RADIATIVE) VIS=0.5 KM
10 - DESERT EXTINCTION, VIS BASED ON WIND SPEED
11 - NOVAM MODEL

ENTER # OF ITEM TO BE SELECTED OR
        0 TO CONTINUE
```

Note that the default boundary layer aerosols have optical properties stored at 0, 1 and 2 km. The extinctions are extrapolated from the stored value at 2 km to zero at 3 km. Also, if Item 3 (NAVY MARITIME EXTINCTION, VIS BASED ON WIND SPEED/HUMIDITY) or Item 10 (DESERT EXTINCTION, VIS BASED ON WIND SPEED) is selected for the boundary layer aerosol, an additional menu allows the user to specify a wind speed from which the visibility is calculated.

The season dependence of the profiles and extinction for the tropospheric (2 to10 km with the extinctions extrapolated to zero at 11 km) are determined by selecting either the spring-summer or fall-winter options in the SEASONAL AEROSOL PROFILE menu, which is accessed by choosing Item 2 in the AEROSOL DESCRIPTION menu:

```
SELECT SEASONAL AEROSOL PROFILE

  1 - SPRING-SUMMER
  2 - FALL-WINTER

ENTER # OF ITEM TO BE SELECTED OR
        0 TO CONTINUE
```

The models for stratospheric aerosols, for which values are stored from 10 to 30 km and extinctions are extrapolated to zero at 35 km, are described below. The models also select the mesospheric aerosols from 30 to 100 km. There are eight models, each combining a vertical altitude profile with an extinction profile that varies with wavelength. Selecting Item 3 AEROSOL DESCRIPTION menu displays the STRATOSPHERIC AEROSOL PROFILE AND EXTINCTION submenu:

```
SELECT STRATOSPHERIC AEROSOL PROFILE AND EXTINCTION

  1 - BACKGROUND STRATOSPHERIC PROFILE  AND EXTINCTION
  2 - MODERATE VOLCANIC PROFILE AND AGED VOLCANIC EXTINCTION
  3 - HIGH VOLCANIC PROFILE AND FRESH VOLCANIC EXTINCTION
  4 - HIGH VOLCANIC PROFILE AND AGED VOLCANIC EXTINCTION
  5 - MODERATE VOLCANIC PROFILE AND FRESH VOLCANIC EXTINCTION
  6 - MODERATE VOLCANIC PROFILE AND BACKGROUND STRATOSPHERIC EXTINCTION
  7 - HIGH VOLCANIC PROFILE AND BACKGROUND STRATOSPHERIC EXTINCTION
  8 - EXTREME VOLCANIC PROFILE AND FRESH VOLCANIC EXTINCTION

ENTER # OF ITEM TO BE SELECTED OR
       0 TO CONTINUE
```

The AEROSOL DESCRIPTION menu also contains options for selecting the Army Vertical Structure Algorithm (VSA) for aerosols in the boundary layer (Item 4) and the surface meteorological range which overrides the default value associated with the selected boundary layer aerosol (Item 5). The last item in the AEROSOL DESCRIPTION menu (Item 6) allows the user to select several options for selecting the aerosol scattering phase function.

The third item in the SUMMARY OF MULTIPLE SCATTERING CALCULATION menu leads to a set of menus to define the cloud MS calculation as shown below:

```
CLOUD MULTIPLE SCATTERING CALCULATION

  1 FOR NO CLOUDS
  2 MODIFY CLOUDS OR INCLUDE RAIN

ENTER # OF ITEM TO BE SELECTED OR
       0 TO CONTINUE
```

Here Item 1 allows the user to remove the clouds and rain from the MS environment. To change the current description of the cloud or rain properties, entering "2" displays the following submenu:

```
MODIFY CLOUD DESCRIPTION

    1 - CUMULUS CLOUD LAYER; BASE=0.66 KM, TOP=3.0 KM
    2 - NO RAIN
    3 - CLOUD MODEL PARAMETERS
        DEFAULT VALUES SELECTED

ENTER # OF ITEM TO BE SELECTED OR
         0 TO CONTINUE
```

Item 1 of the MODIFY CLOUD DESCRIPTION allows the user access to the MODTRAN4 cloud profiles (for a more detailed description of the cloud properties, the user should consult the MODTRAN4 users' manual [Berk et al., 1999]). To illustrate, entering "1" presents the user the available cloud models:

```
SELECT CLOUD TYPE

    1 - CUMULUS CLOUD LAYER; BASE=0.66 KM, TOP=3.0 KM
    2 - ALTOSTRATUS CLOUD LAYER; BASE=2.46 KM, TOP=3.0 KM
    3 - STRATUS CLOUD LAYER; BASE=0.33 KM, TOP=1.0 KM
    4 - STRATUS/STRATOCUMULUS CLOUD LAYER; BASE=0.66 KM, TOP=2.0 KM
    5 - NIMBOSTRATUS CLOUD LAYER; BASE=0.16 KM, TOP=0.66 KM
    6 - 2.0 MM/HR GROUND DRIZZLE
    7 - 5.0 MM/HR LIGHT RAIN
    8 - 12.5 MM/HR MODERATE RAIN
    9 - 25.0 MM/HR HEAVY RAIN
    10 - 75.0 MM/HR EXTREME RAIN
    11 - USER DEFINED CLOUD EXTINCTION AND ABSORPTION
    18 - STANDARD CIRRUS MODEL; 64 MICRON RADIUS ICE PARTICLES
    19 - SUB-VISUAL CIRRUS MODEL; 4 MICRON RADIUS ICE PARTICLES

ENTER # OF ITEM TO BE SELECTED OR
         0 TO CONTINUE
```

Item 2 of the MODIFY CLOUD DESCRIPTION menu can be used to modify the rain rate. The user specified rain rate is used from the ground to an altitude specified by top of the cloud when a cloud is present. When no cloud is present, the rain rate is used from the ground to altitude of 6 km.

```
RAIN RATE (MM/HR)

  1 - NO RAIN (DEFAULT)
  2 - USER DEFINED VALUE

ENTER # OF ITEM TO BE SELECTED OR
        0 TO CONTINUE
```

The final item in the MODIFY CLOUD DESCRIPTION menu permits the modification of default cloud parameters associated with the cloud type, such as, cloud thickness, base altitude, optical properties, and water/ice vertical column density. Selecting Item 3 presents the user with a list of options available through the following menu:

```
MODIFY CLOUD MODEL PARAMETERS

  1 - DEFAULT CLOUD THICKNESS
  2 - DEFAULT CLOUD BASE ALTITUDE
  3 - DEFAULT CLOUD EXTINCTION COEFFICIENT
  4 - CLOUD EXTINCTION REFERENCE WAVELENGTH IS NOT USED
  5 - DEFAULT WATER DROPLET VERTICAL COLUMN DENSITY
  6 - DEFAULT ICE PARTICLE VERTICAL COLUMN DENSITY
  7 - DEFAULT CLOUD/RAIN RELATIVE HUMIDITY
  8 - DEFAULT CLOUD MODEL SPECTRAL HENYEY-GREENSTEIN SCATTERING
      PHASE FUNCTION ASYMMETRY  FACTOR FOR WATER DROPLETS
  9 - DEFAULT CLOUD MODEL SPECTRAL HENYEY-GREENSTEIN SCATTERING
      PHASE FUNCTION ASYMMETRY FACTOR FOR ICE PARTICLES

ENTER # OF ITEM TO BE CHANGED OR
        0 TO CONTINUE
```

Again the user should consult the MODTRAN4 users' manual for a detailed description of the parameter definitions and use.

The third item in the top-level menu, "LOS GEOMETRY (LOS RADIANCE STATISTICS/ SCENE INPUTS)," leads to a set of menus for setting various geometrical parameters as shown below in the second-level menu display:

```
3) REVIEW OR MODIFY LINE-OF-SIGHT GEOMETRY

CURRENT LOS DEFINITION:
1. COORDINATE SYSTEM CENTERED AT GEOGRAPHIC NORTH POLE
2. SUN LOCATION
   SOLAR LATITUDE:   -1.7  LONGITUDE:  304.4 DEGREES
3. SPHERICAL EARTH ASSUMED
4. ABSOLUTE LOS LOCATION SPECIFICATION
   DIRECT INPUT OF LATITUDE/LONGITUDE INFORMATION
5. PATH TYPE IS OBSERVER TO SPACE
   OBSERVER INFORMATION
   OBSERVER ALTITUDE (KM):           183.800
   OBSERVER LONGITUDE (DEGREES):     213.450
   OBSERVER LATITUDE (DEGREES):       65.803

   SOURCE INFORMATION
   TANGENT HEIGHT(S) (KM):            95.970
   LOS THRU LONGITUDE (DEGREES):     198.720
   LOS THRU LATITUDE (DEGREES):       73.772
6. LOS RADIANCE STATISTICS INPUTS

ENTER # OF ITEM TO CHANGE OR
         0 TO CONTINUE
```

Here, Item 1 allows the choice of either the magnetic or geographic pole as the origin of the coordinate system. The point immediately below the sun is established in Item 2; this information is used to determine solar illumination angles during the LOS calculation. In Item 3 the user chooses between a spherical or oblate spheroidal earth. Item 4 distinguishes between two methods for defining the LOS:

- by the latitude, in degrees north of the equator, and longitude, in degrees east of Greenwich, of reference points beneath the LOS (Absolute LOS specification, as shown above), or

- by the solar zenith and azimuthal angles of such reference points (sun-relative LOS specification).

After setting these parameters, the user defines the LOS path in Item 5. Three basic path types are allowed: observer (at some location) to a source point, observer to space (the point where a LOS reaches 300 km altitude is considered space), and limb view (from 300 km to 300 km, passing through a specified tangent height). For each path type, the user is presented with a list of options for defining the path. The options available are constrained by the path type and the earlier choice of

absolute/relative LOS specification. See Subsections 4.3.3 and 4.3.4 below for diagrams showing the geometries for the several path types. These menu options provide flexibility in LOS definition. Cycling through them can enable the user to develop a desired LOS iteratively, using the SAMM geometry package rather than calculating reference points outside the code.

SAMM2 allows the user to perform calculations on a series of basic LOS types to model a 2D scene as observed by a sensor in the upper atmosphere. Item 5 of the second-level LOS GEOMETRY menu can be used to input a series of LOS's for a scene. To illustrate, if a user responds with "5" to the second level menu, s/he gets:

```
PATH TYPES
  2 -- OBSERVER TO SOURCE POINT
  3 -- OBSERVER TO SPACE
  4 -- LIMB VIEWING PATH
  5 -- OBSERVER TO SOURCE PATHS FOR A SCENE
  6 -- OBSERVER TO SPACE PATHS FOR A SCENE
  7 -- LIMB PATHS FOR A SCENE
SELECT PATH TYPE (0 TO KEEP CURRENT INFORMATION)
```

Path types 2, 3 and 4 refer to the basic LOS types discussed in the preceding paragraph. Path types 5, 6 and 7 refer to a multiple number paths of type 2, 3 and 4, respectively, for modeling a scene. For example, if the user tailors the SAMM input file to do a scene calculation using, say, five paths of type 2, upon completion of the process a response of "3" (LOS GEOMETRY) to main menu would result in a second-level display similar to the following:

```
3) REVIEW OR MODIFY LINE-OF-SIGHT GEOMETRY

 CURRENT LOS DEFINITION:
  1. COORDINATE SYSTEM CENTERED AT GEOGRAPHIC NO. POLE
  2. SUN LOCATION
     SOLAR LATITUDE:  -23.0  LONGITUDE:  180.0 DEGREES
  3. SPHERICAL EARTH ASSUMED
  4. ABSOLUTE LOS LOCATION SPECIFICATION
     DIRECT INPUT OF LATITUDE/LONGITUDE INFORMATION
  5. PATH TYPE IS OBSERVER TO SOURCE (SCENE)
     OBSERVER INFORMATION
     OBSERVER ALTITUDE (KM):              425.000
     OBSERVER LONGITUDE (DEGREES):           .000
     OBSERVER LATITUDE (DEGREES):            .000

     SOURCE INFORMATION
     SOURCE ALTITUDE(S) (KM):          30.000    30.000    30.000    30.000
                                       30.000
     ZENITH ANGLE(S) (DEGREES):       120.000   135.000   150.000   165.000
                                      180.000
     AZIMUTH ANGLE (DEGREES):            .000
     SHORT PATH (0) OR LONG PATH (1):       0         0         0         0
                                            0
  6. LOS RADIANCE STATISTICS INPUTS

 ENTER # OF ITEM TO CHANGE OR
        0 TO CONTINUE
```

Here several LOS parameters are multiply listed; each value corresponds to a single LOS. Thus, the five LOS's have zenith angles of 120, 135, 150, 165 and 180 degrees. Each has a source altitude of 30 km and so on.

Item 6 is used to define the LOS radiance statistics parameters. These input options are shown below for a single LOS and include definition of the scan directions in which the user wants radiance statistics.

```
RADIANCE STATISTICS LOS/FOV OPTIONS

  1) CORRELATION LENGTH OPTIONS
     RADIANCE CORRELATION LENGTHS SCALED TO TANGENT POINT
  2) FIELD-OF-VIEW OPTION
     VERTICAL AND HORIZONTAL DIVERGING RAYS
  3) NUMBER OF IMAGE SCANS OPTION
     STATISTICS FOR HORIZONTAL AND VERTICAL SCANS

ENTER # OF ITEM TO BE CHANGED OR
        0 TO CONTINUE
```

Typically the user is interested in horizontal and vertical scans. Menu item 3 for this option is shown below.

```
RADIANCE STATISTICS FOR SCANS ACROSS IMAGE PLANE
  (THERE MUST BE AT LEAST ONE SCAN)

ENTER 0 TO CONTINUE
    1 FOR HORIZONTAL SCAN
    2 FOR HORIZONTAL AND VERTICAL SCANS
    N FOR GRID OF EQUIANGULAR SCANS
      HORIZONTAL, VERTICAL, AND  (N-2)
      INTERMEDIATE SCANS. (N LE  10)
```

The fourth top-level item specifies the spectral interval and the spectral resolution of the output. Also, the radiators to be included in the LOS radiation transport calculation are named. These must be a subset of the radiators treated in the population calculation; a species' contribution to radiance and transmittance cannot be determined if its various population levels have not been calculated!

Item 5 of the top-level menu determines what information will be placed in the output file. The possible options are discussed in Subsection 3.2.9 above.

The sixth top-level item allows the user to choose root names for the output, radiance and transmission files and the directory where they will be placed.

4.3 Input Parameters

This section describes key input parameters for the ambient and auroral populations, LOS geometry and radiation transport modules. The Monte Carlo control parameters used in the ambient populations module warrant further discussion since their values affect the accuracy of this stochastic simulation. Parameters used to define the auroral conditions are discussed in detail. The Geometry parameters section describes the various subsets of geometry variables needed to define an LOS. Finally the parameters used to define the spectral interval, resolution, and species included in the calculation are discussed.

4.3.1 Ambient Population Parameters

The ambient populations module contains a set of routines that determine the enhancement of the species excited-states population profiles due to layer radiative self-trapping and layer-layer radiative pumping. The first-order population enhancement is determined using a Monte Carlo simulation of the initial photon emission and its subsequent absorption or escape. The number of photons determines the statistical uncertainty of the Monte Carlo calculation. Changing this variable to a small number saves computer time, but causes large statistical uncertainties. For reasonable statistical uncertainties the number of photons should be 10,000 or larger.

The maximum order of scattering determines the number of matrix multiplications, Equation (19) of Section 3.2.3, used by NEMESIS to calculate the population enhancement matrix. Changing this number to less than 100 does not save much computer time since the Monte Carlo simulation is performed for first-order scattering only and higher order scattering is determined recursively. Many orders of scattering may be important for some molecular bands, such as 4.3 μm CO_2 radiation. A value of 200 for the maximum order of scattering is sufficiently large.

The remaining parameter governs earthshine pumping, which results from the atmospheric absorption of photons emitted by the hot (~300 K) earth surface. It should be noted that a wavelength independent, totally emissive earth surface is assumed. A value of 1 means the pumping is on, and a value of 0 means the pumping is off.

4.3.2 Ambient Temperature Statistics Parameters

SAMM2 requires a description of the altitude dependent temperature statistics as an input file. The NSS model [Strugala *et al.*, 1993], which is a 1-D non-stationary description of the temperature statistics, is delivered with SAMM2 (file STATS_NSS.DAT). In addition, a validated temperature statistics file (STATS_MSX.DAT), based on recent analyses of MSX limb structure observations, is also provided. There are options available through the interactive input module which allows the user to scale the temperature variance and correlation lengths by constant multiplicative factors. This option is useful for parametric studies on the size of the temperature statistics and their effects on the radiance statistics. The user can also select the vertical and horizontal power spectral indices for the temperature PSD.

4.3.3 Auroral Population Parameters

The model parameters describing an auroral event allow the user to either select a code-supplied aurora or to define a user-specified aurora, as well as to specify the duration of the aurora and observation time. As developed in AARC [Winick *et al.*, 1987], two simple forms for the auroral primary electron spectral flux are available in SAMM2, a Maxwellian flux and a Gaussian flux. The Maxwellian flux is representative of diffuse auroras and is characterized by two parameters, the total energy flux and a characteristic energy (equal to one half the mean energy). The Gaussian flux is characteristic of electron energy spectra in discrete auroras and is defined by three parameters, the total flux, mean energy, and variance of the incident electron energy. However, the user can select three typical auroral electron spectra with a Maxwellian distribution corresponding to IBC classes of II, III, or III$^+$. Finally, the user must select the duration of the aurora, and the observation time relative to the beginning of the electron dosing (which is assumed to be 0 sec). The input units are:

- flux: ergs/cm^2/sec,
- energy: keV,
- time: sec,
- variance: (keV)^2 (for Gaussian flux)

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4.3.4 Local Region Geometry

Auroral excitation is confined to a finite region within the atmosphere. SAMM2 expects separate sets of atmospheric profiles for each local region and for the rest of the atmosphere. Each local region that is auroral has its own set of auroral parameters. The auroral radiance calculation for the specified LOS can be done either during the dosing or at some period subsequent to it by specifying the observation time.

A local region is defined by four (latitude, longitude) points plus the upper and lower altitudes of the region. Only two distinct values are possible for each latitude and longitude components, i.e., Lat_1, Lat_2, Lon_1, Lon_2. The four points must form a convex quadrilateral, which has no interior angles greater than $180°$. The specification of the four points in (altitude, latitude, longitude) coordinates is illustrated in Figure 11. The user should note that the specific clockwise order of the latitude and longitude components, i.e., Lat_1/Lon_1, Lat_2/Lon_1, Lat_2/Lon_2 and Lat_1/Lon_2, as shown in Figure 11, is required for a proper definition of the local region. A coordinate system pole cannot be within a local region. If a pole is to be within an auroral region, the input geometry should use the alternate geographic coordinate system, e.g., use coordinates centered on the geographic pole when the auroral region includes the geomagnetic pole. The altitude profile used for the local region must be extended down to 0 km even though the lower boundary of the region is much higher. This is necessary because the NEMESIS calculation for radiative excitation requires a full profile in order to get the proper upwelling earthshine and layer to layer radiative pumping. For the LOS radiance calculations, SAMM2 uses the populations from the extended region below the region's lower altitude boundary and above the regions upper altitude boundary.

A typical path is illustrated in Figure 11, where each of the path segments has been numbered according to the layer boundaries the path intersects, including the local region boundaries to distinguish portions of path segments inside and outside the local region. Usually the LOS of the radiance calculation only intersects the local region twice. However, because of earth curvature effects, four intersections are possible for a limb path whose minimum altitude is just slightly less than the lower region boundary. For example, a limb path with a tangent altitude of 89 km combined with a lower region boundary of 90 km will have four intersections when the horizontal extent of the region is several hundred kilometers to each side of the tangent point.
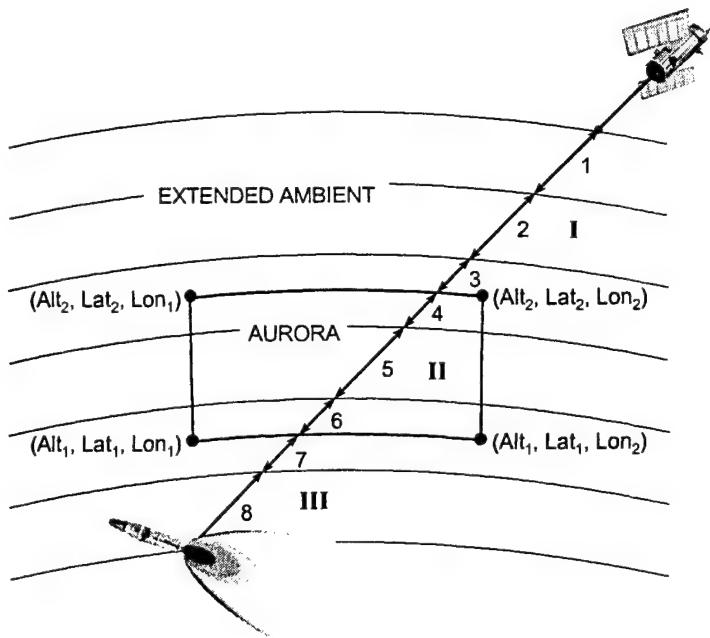
Figure 11. Layering Schematic with Local Auroral Region

4.3.5 Line-Of-Sight Parameters

The LOS is defined as the line that connects the observer located at a point H_1 to the source located at H_2, including curvature of the LOS due to atmospheric refraction. Three basic classes of LOS paths are supported by SAMM2 and are specified through a path parameter:

PATH = 2 -- observer to source,

     = 3 -- observer to space, and

     = 4 -- limb viewing.

The geometry nomenclature is derived from the low-altitude radiance code LOWTRAN 6 [Kneizys *et al.*, 1983]. In the current SAMM2 version, there is no PATH = 1 option. There are a number of geometric parameters that must be specified to define the LOS path, and these are defined in Table 3 and illustrated in Figures 12 and 13. Altitudes and ranges are given in km, and angles in degrees. Longitudes can have values ranging from $0°$ to $360°$ east of Greenwich, and latitudes, from $-90°$ at the south pole to $90°$ at the north pole. A_0 is the local zenith angle of the LOS as measured from the vertical line connecting H_1 and the earth center. The angle B_0 is the azimuth of the LOS measured in degrees east of north from the observer; it varies from $-180°$ to $180°$.
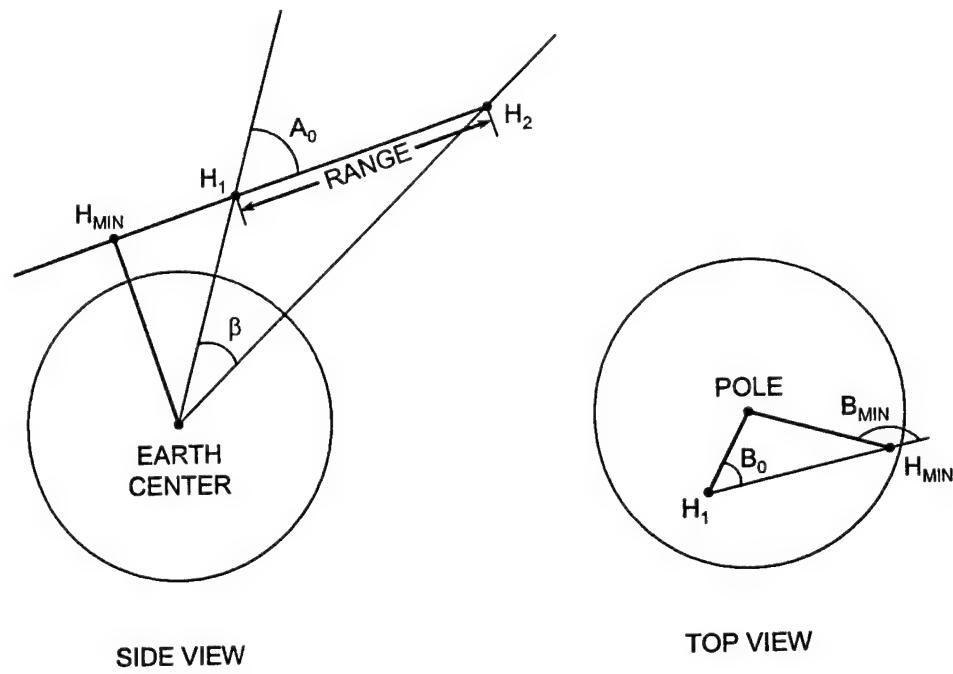
Figure 12. Definitions of LOS Angles, Range, and Altitudes.
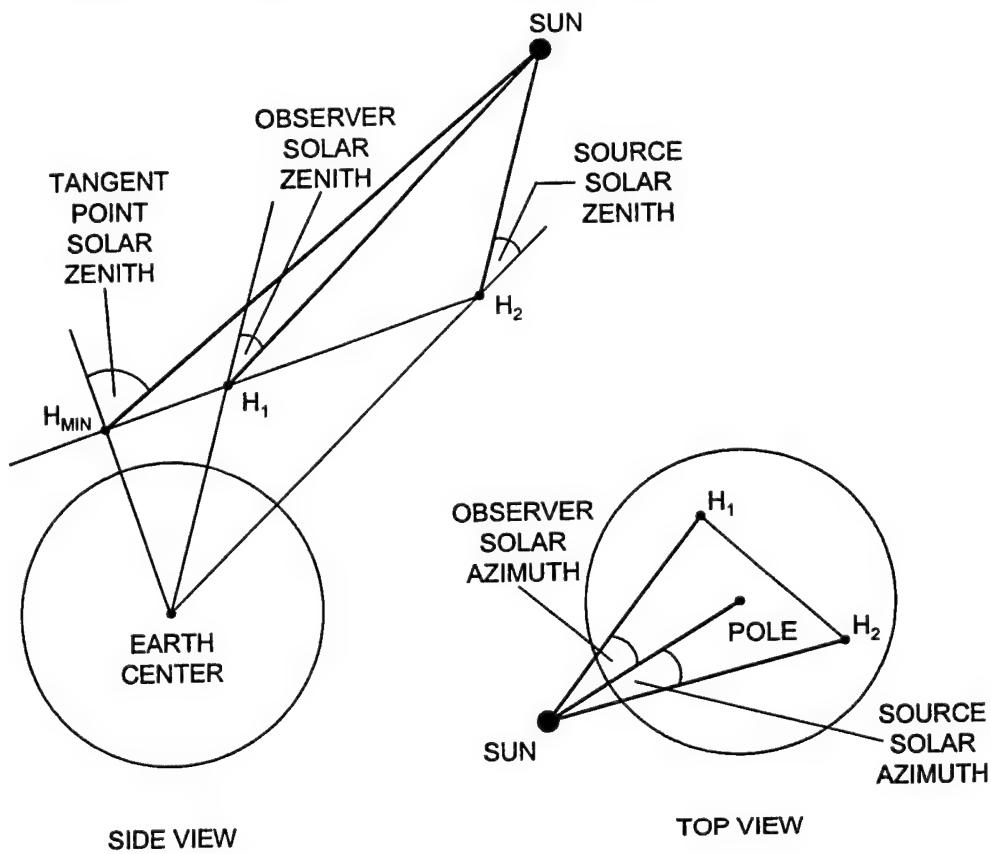
Figure 13. Definition of LOS Solar Angles.

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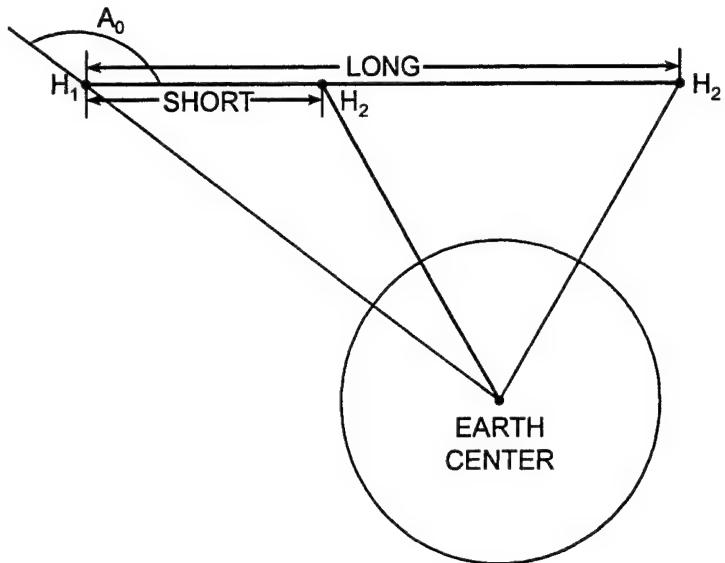
Figure 14. Illustration of Short and Long LOS Down-Looking Paths.

The parameters listed in Table 3 over specify the LOS. For a particular LOS only one of many different subsets is required as input. The other parameters are calculated internally. Each class, designated by its PATH value, has various options for specifying the LOS. These are labeled by CASE and are listed in Table 4 along with the required geometrical inputs. The particular case with PATH = 2 and CASE = 1 can be ambiguous when observer altitude is greater than the source altitude and the LOS zenith, A_0, is greater than 90°. This is a down looking scenario in which the source point is either before the tangent point (short) or past the tangent point (long). SAMM2 allows observer to space LOS for which the observer is either up looking or down looking. Thus the LOS must be specified short or long whenever using the PATH = 3 and CASE = 2 option. Two paths distinguished by LOS = (short, long) are illustrated in Figure 14.

The definition of the LOS will change if the user switches between the spherical earth and the oblate spheroidal earth options. The LOS definition changes because the radius of the earth changes. The variables have the same meaning, but their values may change.

Table 3. LOS Parameters.

SOLAR LOCATION (SUN)
  longitude
  latitude
OBSERVER POINT PARAMETERS (H_1)
  altitude
  longitude
  latitude
  solar zenith
  solar azimuth (pole-sun-observer)
SOURCE POINT PARAMETERS (H_2)
  altitude
  longitude
  latitude
  solar zenith
  solar azimuth (pole-sun-source)
TANGENT POINT PARAMETERS (H_{min})
  altitude
  longitude
  latitude
  solar zenith
  solar azimuth (pole-sun-tangent point)
ARBITRARY POINT PARAMETERS (H_p)
  longitude
  latitude
  solar zenith
  solar azimuth (pole-sun-point)
LOS LENGTH AND ORIENTATION PARAMETERS
  RANGE, the distance from observer to source, H_1 to H_2
  LOS paths which do not include the tangent point are <u>short</u>.
  LOS paths which do include the tangent point are <u>long</u>.
  BETA, the earth-center angle between H_1 and H_2
  A_0 the zenith angle of LOS at observer
  B_0, the (pole-observer-LOS) azimuthal angle;
  B_{min}, the (pole-tangent point-LOS) azimuthal angle;
Note: All azimuths defined as (north = 0° & east = 90°).

Table 4. Geometry Input Sequences.

PATH	CASE	Geometrical Inputs
2	1	H_1, H_2 (altitude), A_0, B_0
		H_1, H_2 (altitude), A_0, B_0, (short/long)
	2	H_1, RANGE, A_0, B_0
	3	H_1, H_2 (altitude), RANGE, B_0
	4	H_1, H_2 (altitude), BETA, B_0
	5	H_1, H_2
3	1	H_1, A_0, B_0
	2	H_1, H_{min} (altitude), B_0, (short/long)
4	1	H_1, H_{min}, B_{min} (short/long)
5	1	H_1, H_2, (altitude), several A_0's, B_0
		H_1, H_2, (altitude), several A_0's, B_0, (sort/long)
	2	H_1, RANGE, several A_0's, B_0
6	1	H_1, several A_0's B_0
	2	H_1, several H_{min}'s (altitude), B_0, (short/long)
7	1	H_1, several H_{min}'s (altitude), B_{min}, (short/long)

Note:

1. There are two ways to enter the point H_1.
   (1) H_1(altitude, latitude, longitude) or
   (2) H_1(altitude, solar zenith, solar azimuth)
   for absolute or relative specification respectively
   H_2 and H_{min} are defined analogously.

2. There are three ways to input the observer LOS azimuth angle B_0:
   (1) direct entry in degrees,
   (2) defining a point along the LOS trajectory before H_1
   (3) defining a point along the LOS trajectory after H_1

3. There are three ways to input the tangent point azimuth angle B_{min}:
   (1) direct entry in degrees,
   (2) defining a point along the LOS trajectory before H_{min}
   (3) defining a point along the LOS trajectory after H_{min}

4. Paths 5, 6 and 7, are intended for multiple LOS inputs, and are similar to 2, 3 and 4, respectively.

5. Where multiple zenith angles (A_0's) are required, they are computed from these inputs: boresight angle (angle at mid FOV), an increment and total number of LOS's

6. Where multiple H_{min} altitudes are required, they are computed from two different sets of inputs:
   (1) minimum and maximum bounding H_{min} values and total number of LOS's
   (2) minimum, maximum and an intermediate H_{min}'s, plus two increments between the minimum and the intermediate H_{min}, and between the intermediate and the maximum H_{min}

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4.3.5.1 Forcing the LOS to Intersect Regions

One of the uses of the arbitrary point option (H_p) for specifying the LOS azimuth angles is to orient the LOS so that it intersects a particular region. If the point option is used, specifying the point latitude and longitude within a local region will force the LOS to intersect the region if it passes within the upper and lower region altitude. Another use of the arbitrary point option is to control the change in zenith angle over a given LOS. For example, by specifying the same solar zenith angle for both the arbitrary point along the LOS and the source, the LOS would have a constant solar zenith angle, i.e. the LOS would be parallel to the solar terminator.

4.3.5.2 LOS Statistics Options

There are several parameters which relate the sensor/observer image plane to the LOS characteristics for a given SAMM2 calculation. The statistical correlation lengths for the radiance must be projected onto some point along the LOS. Typically, in limb calculations the correlations lengths are reported for the LOS tangent point. For non-limb LOS's the point along the LOS at which the correlation lengths are determined is more arbitrary. The LOS reference point is specified as a range from the observer, or as the minimum altitude point along the LOS path. The user can also select diverging or parallel rays from the sensor. The rays are parallel for a sensor placed at infinity. For most scenarios the diverging rays option is appropriate.

The user can also specify the directions across the image plane for which statistical radiance calculations will be performed. Generally the image plane horizontal and vertical are of interest, but diagonal scans across the image plane may also be of interest. This option is selected by choosing the number of scans for calculation. An answer of one determines only the horizontal radiance statistics, two will determine both horizontal and vertical, while an answer of three or larger leads to the determination of radiance statistics for n-2 diagonal scans with incremental angles of 90 degrees/(n-1) off the vertical, e.g. for n=4 the two diagonal scans would be for 30 and 60 degrees off vertical.

4.3.6 Spectral Radiance Parameters

The spectral range is defined by specifying the minimum and maximum frequency (cm^{-1}) of interest. SAMM2 currently includes lines from 250 to 5000 cm^{-1}. for all species except OH, which includes lines additional lines from 5000 to 10000 cm^{-1} for the OH(Δv=3-6) transitions. The maximum spectral resolution is 0.001 cm^{-1}. Currently, the spectral radiance array contains at most 50,000 points. So, if a resolution of 0.001 cm^{-1} is specified, only a 50 cm^{-1} spectral interval can be used. If the user specifies a spectral resolution greater than 0.002 cm^{-1}, a triangular slit function with a full-width, half-maximum equal to the input spectral resolution is used to degrade the spectral output. The spectral resolution parameter is also used as the spectral output step size. Thus, for a spectral resolution of 0.1 cm^{-1}, a spectral range of 5000 cm^{-1} can be specified. The interactive input module will alert the user if the interval is too large for the selected resolution and then reset the maximum frequency to reduce the interval.

The user must specify the species desired for the radiance calculation. The list may be equal to, or a subset of the species contained in population calculations or population files. The species are entered through the interactive input module by typing in their chemical formulas. At the end of a calculation the total number of spectral lines are summarized for each band and species in the general SAMM2 output file.

5. SAMM2 OUTPUT FILES

The user can control the amount of SAMM2 output to suit the need at hand by responding with "5" to the main interactive menu. Upon the response, SAMM2 will display the following second-level menu:

```
5) REVIEW OR MODIFY OUTPUT DESIRED...

    IWRITE VALUES RANGE FROM 0 TO 3
    LOW VALUES DECREASE THE AMOUNT OF OUTPUT
    HIGH VALUES INCLUDE ALL OUTPUT FROM LOWER VALUES
    FOR EXAMPLE: IWRITE=2 WOULD INCLUDE IWRITE=1 OUTPUT

    CURRENT VALUES ARE:
    1. MODEL ATMOSPHERE OUTPUT:                      0
    2. SELECTED TRANSITIONS:                         0
    3. MOLECULAR BAND INFORMATION:                   0
    4. TEMPERATURE STATISTICS OUTPUT:                0
    5. NEMESIS OUTPUT:                               2
    6. AURORAL OUTPUT:                               0
    7. FINAL EXCITED STATE POPULATIONS:              0
    8. EXCITED STATE VIBRATIONAL TEMPERATURES:       0
    9. LINE-OF-SIGHT OUTPUT:                         0
    10. SPECTRAL RADIANCE OUTPUT:                     0
    11. RADIANCE STATISTICS OUTPUT:                   2
    12. RADIANCE COVARIANCE MODEL:                    1
    13. FILES FOR 2D AND 3D SCENE GENERATION:         1

ENTER # OF ITEM TO BE CHANGED OR
        0 TO CONTINUE
```

In the following the contents of the SAMM2 output files are described. Also described is how the user can create these files by choosing the appropriate integer value for the above 13 choices.

5.1 Journal File

The SAMM2 journal file (SAMM2.LOG) contains various informational statements generated during SAMM2 execution. The majority of messages are due to problems encountered with parameters in the input files. Warning or caution messages usually result from inconsistent use of input files. An error message during execution is considered fatal, and execution will stop after the

error message is written to the journal file. A warning or caution message is not fatal (that is, does not terminate execution), but it should inform the user that input files are inconsistent, that only a partial calculation has been performed, or that numerical difficulties have been encountered and fixed in one of the SAMM2 modules. The user should monitor the journal file after each SAMM2 run to insure that the desired calculation was properly performed. During auroral calculations, several warning messages are routinely given stating that different molecular species were not found. Since auroral excitation is only calculated for CO_2, NO, and NO^+, these messages are reasonable, but the user should check that these species were not inadvertently omitted too.

There are over 150 different error/caution messages that can be written during execution. These messages contain the name of the subroutine in which the problem occurred. For example, consider an error resulting from inconsistent input in the molecular states and bands files (see Subsections 6.2 and 6.3, respectively). Assume that the $2 \rightarrow 1$ vibrational transition for CO has been specified in the molecular states file (see Table 8 in Section 7). If the data for the line strength distribution function for the $2 \rightarrow 1$ transition have not been included in the molecular bands file (see Table 9 in Section 7), the following error message will be written to the journal file:

ERROR IN BANDIN...

CO(2)   - CO(1)   BAND MISSING FROM BAND DATA

prompting the user to check the CO bands file for either an input error or omission of data.

As seen in this example, the error/caution messages generated from the input files are usually self-explanatory, and the user should be able to easily correct the problem. In some cases, however, the problem may be more subtle. For example, messages generated during calculation of number densities of vibrationally excited states most likely will require the user to carefully check the chemical kinetics mechanism and the list of transitions considered by the ambient populations module.

5.2 General Output File

The general SAMM2 output file contains a summary of selected output from each module. As mentioned previously, three levels of output (0,1,2) can be obtained from each SAMM2 module. The level (and amount) of output is selected through the interactive menu (see Subsection 3.2.9). The level of output is controlled independently for various modules. The lowest level contains the minimum amount of information (level = 0) necessary to characterize the calculation, and the highest level contains the maximum amount of information (level = 2). The information written to the output file for the level options is illustrated in Table 5. Notice that the atmosphere name and the band radiance summary are always written to the output file, and the spectral radiance as a function of frequency is always written to the spectral file.

5.3 Population File

For a given set of species and kinetic schemes, the excited-state populations for each atmospheric layer change only when atmospheric conditions change; some examples are a new model atmosphere, day and night conditions, new solar zenith angle, or auroral conditions. The excited-state populations and the information necessary to characterize them uniquely are written to a binary "population" file. This allows the user to perform multiple SAMM2 calculations for any number of observer-source scenarios without re-calculating the populations each time. The relevant information written to the "population" file is:

- Name of the model atmosphere file (Subsection 6.6),
- Names of the molecular radiators and the associated "linking", "states", and "bands" files,
- The species listed in the chemical kinetics input ("linking") files (Subsection 7.1) for each molecular radiator,
- The molecular states file (Subsection 6.2) for each molecular radiator,
- The molecular state populations, population fluctuations and associated temperatures for each radiator, and
- The auroral parameters when the auroral option is used.

Table 5. Type of Output Contained in SAMM2.OUT File.

OUTPUT	OPTION	DESCRIPTION
Model Atmosphere	0	Atmosphere file name
	1,2	Complete atmospheric input file
Selected Transitions	0	No output
	1,2	Complete molecular states input file
Molecular Band Data	0,1	No output
	2	Complete molecular bands input file
Temperature Statistics	0	No output
	1	Complete temperature statistics file
Ambient Output	0	No output
	1	Initial steady state layer source populations and nemesis excited state population enhancements; earthshine, sunshine, and excitation rates; and the quenching/re-emission probabilities
	2	Post NEMESIS excited state populations for each selected transition
Auroral Output	0	No output
	1	Final population for all auroral species
	2	Populations of all auroral species as a function of time
Final Excited State Populations	0	No Output
	1,2	Final excited state populations
Final Excited State Temperatures	0	No Output
	1,2	Final excited state temperatures
Line of Sight Output	0	No Output
	1,2	Species total column densities along line of sight
Spectral Radiance Output	0	Plot file (SAMM2.SPC)
	1,2	Spectral radiance table
Radiance Statistics Output	0	Summary in general output
	1	Numerical covariance file
	2	Additional LOS dependent quantities
Radiance Covariance Output	0	No Output
	1	Modified Bessel Function Approximation to Radiance Covariance
2D and 3D Scene Generation	0	No Output
	1	Generate files for 2D and 3D scene generation

For subsequent calculations with the same "population" files, it is only necessary to change the input and output parameters relevant to the LOS specification and/or radiation transport sections of the SAMM2.INP file (Subsections 4.2 - 4.3). Although the complete set of options listed in Table 5 for the amount of detail in the general output file are not available when using a previously created population file, the output file does contain sufficient detail to characterize uniquely the population file used. However, the user should refer back to the original general output file generated when the population file was created if greater detail is desired.

5.4 Spectral Radiance File

An ASCII file is created to allow the user either to plot the calculated spectral radiance directly or to modify/reduce the results further. For example, the user may wish to apply a specific filter function to the spectral radiance or to convert to a set of units other than those used by SAMM2. The plot file contains two columns with the frequency (cm^{-1}) and the spectral radiance ($W/sr/cm^2/cm^{-1}$) written as an (x,y) ordered pair.

5.5 Band Radiance File

An ASCII file is created to allow the user either to conveniently access or plot the band radiance in the spectral range defined by the minimum and maximum frequency directly without referring to the general output file. This file is most convenient when the multiple LOS option has been selected. The file name is formed by concatenation of the output file root name with an identifying extension, in this case .BRD. For example, if the output file is named TEST1.OUT then the band radiance file is automatically named TEST1.BRD. The file contains four columns containing the band radiance ($W/sr/cm^2$), tangent height (km), sensor zenith angle (degrees), and LOS number.

5.6 Spectral Transmittance File

An ASCII file is created to allow the user either to plot the calculated spectral transmittance directly or to modify/reduce the data further. For example, the user may wish to apply a specific filter function to the transmittance or to convert to a set of units other than those used by SAMM2. The plot file contains two columns with the frequency (cm^{-1}) and transmittance written as an (x,y) ordered pair.

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5.7 Other Files in the Population File Directory

If the statistical structure calculation is selected, there are two additional sets of files which are created in the population file directory. These files, which are from the NEMESIS calculation, contain the response of the vibrational state number density and temperature to the variation in kinetic temperature for each molecular isotopic radiator. The files are identified by the extension .CV1 and .VT1 for the vibrational number density and temperature, respectively. For example, if one performed a calculation with only the major isotope of CO_2 and the population file was named POPSADAY.000, the CV1 and VT1 files would be called POPSADAY.000CO21.CV1 POPSADAY.000CO21.VT1, respectively.

These files, which are created by choosing the second-level menu item 5 [NEMESIS OUTPUT] in the main interactive menu [5) REVIEW OR MODIFY OUTPUT DESIRED...] to be greater than or equal to 2, are briefly described below.

5.7.1 The Vibrational Number Density Response File

For each molecular vibrational ground and excited state, the first order response in number density to a unit kinetic temperature fluctuation is given for each altitude layer in the atmospheric profile. The first record has the number of layers and number of molecular states of the radiator. The next records contain the HITRAN notation for the molecular states. Then for each altitude layer, the altitude and the responses of the molecular states are given. These files have the extension .CV1.

5.7.2 The Vibrational Temperature Response File

For each excited vibrational state the first order response in vibrational temperature to a unit kinetic temperature fluctuation is given for each altitude layer in the atmospheric profile. The format of these files is identical to the CV1 files with the exceptions that one less molecular state is included (the ground state is excluded), and the responses are for vibrational temperature rather than number density. These files have the extension .VT1.

5.8 Other Files in the Output Directory

These files are found in the output directory. The names are formed by concatenation of the output file root name with an identifying suffix. For example, if the output file is named TEST2.OUT, then the user can request the volume emission output file, TEST2.VMIS, containing the contributions to the total radiance from each segment along the line-of-sight, by setting second-level menu item 10 (SPECTRAL RADIANCE OUTPUT) in the main interactive menu [5] REVIEW OR MODIFY OUTPUT DESIRED...] equal to 2. The VMIS file contains four columns containing, respectively, the radiance contribution ($W/sr/cm^2/km$) from, the distance (km) along, and the lower and upper altitudes (km) of each LOS segment.

Similarly, the "interface" files which contain the 2D and 3D radiance structure information for the SIG scene generator are automatically named TEST2.2D and TEST2.3D, respectively. These files, which are created by choosing the second-level menu items 11 [RADIANCE STATISTICS OUTPUT], 12 [RADIANCE COVARIANCE] or 13 [FILES FOR 2D AND 3D SCENE GENERATION] are described below.

5.8.1 The Radiance Statistics Files

Chose the second-level menu item 11 (RADIANCE STATISTICS OUTPUT) to be greater than or equal to 1 for these files.

These files contain, for each LOS, the SAMM2 prediction of the horizontal and sensor vertical radiance covariance function as a function of lag angle in radians (extension .COVA) or lag distance in kilometers (extension .COVD). Output for each LOS is delimited with a record containing the LOS number, the tangent point altitude and the sensor altitude and zenith angle. At the end of each tabulated radiance covariance function, there is a record which identifies the off-horizontal angle in radians, 0. for horizontal and 1.57 for sensor vertical.

5.8.2 The Radiance Variance Distribution Function File

Set the second-level menu item 11 (RADIANCE STATISTICS OUTPUT) to 2. This will produce the variance distribution function VDIS file, in addition to the COVA and COVD files.

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The VDIS file contains three columns. The first column is the radiance variance distribution function ($\{W/sr/cm^2\}^2/km$), which determines the weighting or contributions to the radiance variance from each segment along the LOS. Integration of the variance distribution function along the LOS yields the radiance variance. The radiance variance distribution function is tabulated together with the altitude (km) of the LOS segment midpoint (second column) and the range (km) from the sensor to that point (third column). Output for each LOS is delimited with a record containing the LOS number, the tangent point altitude and the sensor altitude and zenith angle. At the end of each tabulated distribution function is a record containing the radiance standard deviation.

5.8.3 The Radiance Covariance Model File

To create this file, set the second-level menu item 12 (RADIANCE COVARIANCE MODEL) to 1.

SAMM2 estimates the spectral slope of a radiance covariance function by performing a non-linear least squares fit of the radiance covariance function to a modified second order Bessel function model of covariance. The BES file contains the resulting model evaluated at the points tabulated for the radiance covariance function. The format of this file is identical to the COVD file except that at the end of each tabulated modified Bessel function approximation is a record which contains the estimated spectral index and the correlation length.

5.8.4 The SIG 2D and 3D Files

To create these two files, set the second-level menu item 13 (FILES FOR 2D AND 3D SCENE GENERATION) to 1.

These files serve as interface between SAMM2 and SIG, the SHARC/SAMM Image Generator. The files contain headers which identify the conditions and options used to generate the output. The header includes the selected bandpass, the temperature statistical model parameters, and the sensor altitude. In the 2D file, following the header is a record for each LOS which contains the tangent altitude (km), sensor zenith angle (degrees), the source range (km), the "image plane range" (km), the mean radiance ($W/cm^2/sr$), the standard deviation of radiance normalized by the mean ($W/cm^2/sr$),

horizontal and vertical correlation angles (radians) or distances (km), and horizontal and vertical spectral indices. The "image plane range" defines a distance from the sensor so that distances and correlation lengths can be assigned to the image as well as angular quantities defined by the FOV.

In the 3D file, following the header are several records for each LOS. The first record specifies the tangent point altitude (km) and source or target altitudes (km), the second specifies the LOS and image plane ranges (km) from the sensor, and the third specifies the number of segments on the LOS for which data is tabulated. The tabulated data, immediately following the third record, consist of the apparent volume emission ($W/cm^2/sr$), the apparent radiance response or fluctuation amplitude ($W/cm^2/sr/km/K$), the altitude of the midpoint of the segment (km), the local elevation angle (degrees) of the LOS at the segment, the accumulated range (km) from the top the atmospheric profile to the end of the segment (km), and the mean profile temperature (K) of the segment.

6. SAMM2 DATA FILES

The particular species, isotopes, states, transitions, concentration profiles, and reaction schemes used by SAMM2 to determine atmospheric radiance and transmission are not built into the code. They are specified by the user through input data files. A basic set is supplied for the SAMM2 radiators. A radiator is defined as a particular isotope of a chemical species (e.g. the three isotopes of CO_2, or major isotope of O_3). Four files are supplied for each radiator which together define the relevant species dependent chemistry. These are the kinetics/linking, states, bands, and low-altitude transmittance files. In addition, the vertical concentration profiles of all species at a given location are set in the model atmosphere files. Four solar irradiance files are included to provide the solar flux for molecular excitation and solar scattering. Surface (ground) reflectivity files are provided to characterize the spectral albedo for various material types. In addition, two sample files are provided to define parameters for several BRDF models over a limited infrared frequency range. Finally, two temperature statistics file are provided to define the parameters necessary for the NSS temperature statistics model. The user may use these files as shipped, but may also modify the chemistry, solar irradiance, ground definition or temperature statistics by changing the files. To permit such modifications, their structures are described below.

6.1 Kinetics Files

The populations for the various vibrational levels of the radiating species are calculated with a kinetic model using rate equations for the important processes. Each species is treated separately. As discussed above, SAMM2 does not have a particular kinetics model built into the software. The user specifies the important reactions for each molecular radiator through its kinetic file. This file contains a description of all the reactions in the model, written in an ASCII format as a kineticist would write them. An important auxiliary program, the INTERPRETER, reads these files and translates them into an ASCII linking file which is read and used by SAMM2 itself. It should be emphasized that a default set of kinetics files for all SAMM2 species is provided for the user. If no changes are made to the kinetics files, the user can simply use these files directly as provided. It is not necessary to run the INTERPRETER if the provided chemical kinetics models are used.

A number of considerations apply when the kinetics files are created or modified. The required information, the flexible formats and the INTERPRETER program are discussed in Subsection 7.1 below.

6.2 Molecular States Files

The molecular states files supply the following information to SAMM2:

- Identification of the molecular radiator;

- Definition of the vibrational energies and degeneracies associated with the vibrational states included in the chemical kinetics mechanism; and

- Definition of the vibrational transitions (that is, molecular bands) which will be treated by NEMESIS and SPCRAD. Note that a transition may be considered by NEMESIS but not by SPCRAD.

The molecular states file is written in ASCII format. The information is stored in all 80 columns and is format free. The SAMM2 CO molecular states file is given in Table 6. As the structure of the molecular states file is described, the reader should refer back to Table 6 as an example of the file organization.

The first line in the states file identifies the radiating species (which must be the first entry on this line). Any subsequent information on this line is treated as a comment and ignored by the code. The next line must contain the identifier ENERGIES starting in Column 1 and thus signals the start of the list of vibrational-state energies and degeneracies. This line is followed by any number of lines, each of which must contain three numbers to identify the particular vibrational state (using the standard HITRAN notation), the energy of that state (in cm^{-1}), and the degeneracy of that state, respectively. Numbers must be separated by at least one blank, and they may be integer, floating point or exponential. After all vibrational states have been listed, the next line must contain the word END beginning in Column 1.

The next section of the molecular states file lists information about the vibrational transitions. The first line following the END line must contain the word TRANSITIONS starting in Column 1. This line is followed by as many lines as necessary to identify: each vibrational transition considered by NEMESIS, and whether or not to compute the radiance along the observer LOS for the transition. The vibrational transition is listed as "U-L" where "U" denotes the upper state and "L" denotes the lower state for the transition. The minus, "-", is the delimiter which separates the upper and lower states in the transition. It is important to note that a transition in the molecular states file must have the corresponding radiative relaxation and excitation processes listed in the chemical kinetics mechanism (compare Table 13 of Section 7 below, and Table 6 below). The LOS radiance option is defined as follows:

- 0 - Radiance is not computed for this transition,
- 1 - Radiance is computed for this transition.

Although the radiance may not be computed for a particular transition, it may be important for the NEMESIS calculation to include the transition in the states file. Each entry, vibrational transition and LOS radiance option must be separated by at least one blank. After all the vibrational transitions information has been given, a line containing the word END beginning in Column 1 must follow.

Table 6. SAMM2 CO Molecular States Input File

```
CO VIBRATIONAL STATES AND TRANSITIONS
ENERGIES AND DEGENERACIES
0            0.000              1
1            2143.272           1
2            4260.063           1
END
TRANSITIONS
1-0          1
2-0          1
2-1          1
END
```

6.3 Molecular Bands Files

The molecular bands files are used to input line strength information for the ambient population module. Bands files are not used in the auroral calculations. This information is used to obtain the

altitude-dependent earthshine and sunshine excitation rates and to calculate the enhancement of molecular excited-state populations due to radiative trapping and atmospheric emission.

Although the ambient population module could use the modified HITRAN line compilation directly, this would be extremely time consuming due to the large number of lines. It is much more efficient to discretize the line strength distribution for each molecular vibrational transition. First, the maximum line strength, S_{max}, for a given molecular vibrational transition is determined. Line strength bins (15 bins are currently used) are then constructed according to the sequence $\{(S_{max}, S_{max}/\sqrt{10}), (S_{max}/\sqrt{10}, S_{max}/10), \dots (S_{max}/10^7, S_{max}/\sqrt{10^{15}})\}$. The spectral lines for a particular vibrational transition are then histogrammed according to their line strength, and the total number of lines assigned to each line strength bin is recorded. An effective line strength equal to the average line strength of all the lines in the bin is determined, and a degeneracy equal to the number of lines used in computing the average line strength is assigned to the bin. In the limit of infinitesimal width bins the exact line strength distribution is recovered. For reasonable choices of bin widths and number of bins, the number of lines that need be considered can be reduced by several orders of magnitude without significant loss of computational accuracy.

The molecular bands file indicates the vibrational transition along with the number of lines in a bin, and the average line strength in the bin at the specified temperature. This information suffices to completely characterize the discretized line strength distribution at each temperature. The file is written in ASCII format using all 80 columns and is format free. The molecular bands file for CO is given in Table 7. Again, the reader should refer back to Table 7 as an example of the file organization.

Table 7. SAMM2 CO Molecular Bands Input File

CO	BAND TRANSITIONS FOR ISOTOPE NUMBER 1						
	1-	0	G	SBAR	SBAR	SBAR	SBAR	SBAR
			5	200.	250.	300.	500.	1000.
			23	0.375E-18	0.352E-18	0.329E-18	0.254E-18	0.149E-18
			9	0.109E-18	0.138E-18	0.161E-18	0.198E-18	0.169E-18
			5	0.324E-19	0.605E-19	0.890E-19	0.167E-18	0.189E-18
			4	0.111E-19	0.265E-19	0.459E-19	0.119E-18	0.171E-18
			4	0.387E-20	0.116E-19	0.234E-19	0.823E-19	0.149E-18
			4	0.120E-20	0.461E-20	0.110E-19	0.541E-19	0.126E-18
			4	0.330E-21	0.167E-20	0.477E-20	0.338E-19	0.104E-18
			3	0.919E-22	0.612E-21	0.210E-20	0.215E-19	0.868E-19
			3	0.326E-22	0.266E-21	0.105E-20	0.141E-19	0.699E-19
			2	0.111E-22	0.115E-21	0.532E-21	0.973E-20	0.604E-19
			4	0.349E-23	0.455E-22	0.245E-21	0.617E-20	0.491E-19
			2	0.871E-24	0.154E-22	0.101E-21	0.372E-20	0.391E-19
			2	0.353E-24	0.749E-23	0.556E-22	0.264E-20	0.334E-19
			3	0.112E-24	0.299E-23	0.259E-22	0.169E-20	0.277E-19
			5	0.205E-25	0.746E-24	0.801E-23	0.821E-21	0.191E-19
END								
	2-	0	G	SBAR	SBAR	SBAR	SBAR	SBAR
			5	200.	250.	300.	500.	1000.
			22	0.294E-20	0.274E-20	0.255E-20	0.195E-20	0.118E-20
			10	0.890E-21	0.112E-20	0.130E-20	0.158E-20	0.138E-20
			5	0.245E-21	0.458E-21	0.674E-21	0.127E-20	0.151E-20
			5	0.775E-22	0.189E-21	0.333E-21	0.898E-21	0.139E-20
			4	0.225E-22	0.714E-22	0.150E-21	0.573E-21	0.116E-20
			3	0.773E-23	0.307E-22	0.745E-22	0.381E-21	0.955E-21
			4	0.257E-23	0.130E-22	0.372E-22	0.265E-21	0.847E-21
			3	0.734E-24	0.491E-23	0.169E-22	0.173E-21	0.733E-21
			3	0.240E-24	0.197E-23	0.779E-23	0.106E-21	0.552E-21
			3	0.736E-25	0.795E-24	0.377E-23	0.737E-22	0.505E-21
			2	0.254E-25	0.336E-24	0.183E-23	0.473E-22	0.400E-21
END								
	2-	1	G	SBAR	SBAR	SBAR	SBAR	SBAR
			5	200.	250.	300.	500.	1000.
			22	0.755E-18	0.711E-18	0.667E-18	0.515E-18	0.303E-18
			9	0.220E-18	0.277E-18	0.322E-18	0.395E-18	0.333E-18
			6	0.635E-19	0.109E-18	0.156E-18	0.282E-18	0.314E-18
			5	0.206E-19	0.497E-19	0.867E-19	0.230E-18	0.337E-18
			3	0.714E-20	0.216E-19	0.439E-19	0.157E-18	0.286E-18
EN=								

The first line in the bands file identifies the molecular species (which must be the first entry on this line) for which the file has been created. Subsequent information on this line is treated only as a comment and is ignored by the code. The molecular species is checked against the radiating species identified in the molecular states file to ensure a consistent set of files is being used. The second line

contains the vibrational transition which is then followed by a list of headings for the columns beneath; "G" indicates the number of lines in the bin, and "SBAR" means the corresponding average line strength. As in the molecular states file, the vibrational transition is listed as "U-L" where "U" denotes the upper state, and "L" denotes the lower state for the transition. The minus, "-", is the delimiter which separates the upper and lower states in the transition. Each transition listed in the molecular states file must have a corresponding entry in the molecular bands file. The next line notes the number of temperatures and the temperatures at which the strength distribution was calculated. The following lines describe the line strength distribution. Each line contains the number of lines in that energy bin and the average line strength at each temperature. (The average line strengths are interpolated to a line strength for each atmospheric layer temperature using a linear interpolation.) The entries must be in the following order:

1. the number of lines in the bin,
2. the average line strength in the bin (cm^{-1}/molecule/cm^{-2}) at T_1,
3. the average line strength in the bin (cm^{-1}/molecule/cm^{-2}) at T_2 continuing up to the nth temperature.

After all the line strength bins have been listed for the particular transition, the next line must contain the word END beginning in Column 1.

6.4 Low Altitude Continuum Transmittance Files

These files are needed when the LOS passes through regions of the atmosphere for which the LOS solar zenith is between $90°$ and $108°$. Use of multiple atmospheric profiles, each representing a different solar zenith, is optional. SAMM2 interpolates between multiple atmospheric profiles to best represent the atmospheric conditions for each segment along the LOS. For angles above $≈108°$ the SAMM2 atmosphere is below the terminator and no solar pumping of the SAMM2 atmosphere is occurring. The nighttime atmosphere is appropriate and no continuum transmittance file is required. When the solar zenith is between $90°$ and $108°$, the atmosphere is pumped by solar radiation that has passed through parts of the lower atmosphere where continuum sources may be important. Since some of this radiation is absorbed by the lower atmosphere, it cannot be represented by an unfiltered solar spectral distribution. The amount of absorption at any wavelength is determined by the solar zenith angle, or equivalently the minimum altitude through which the sunlight passes, and by the aerosol content of the lower atmosphere.

SAMM2 models the attenuation of solar irradiance by "continuum" sources using precalculated transmittances. Here the term continuum denotes all absorbers other than the particular chemical species for which solar excitation rates are being calculated. For each vibrational band, lower atmosphere (< 50 km) continuum transmittances are stored for three aerosol profiles and five solar zenith angles, a total of 15 values. Part of the data for the v_1 band of CO are presented in Table 8. As before, the first line identifies the molecular species. The second line identifies the vibrational transition and its frequency. The third line of the table contains the sines of the solar zenith angles at 50 km altitude. For 50 km solar zenith angles exceeding $97.029°$ [$\sin(97.029°) = .99248427$], the refractive path intersects the earth. The three lines of data which follow in the table (above the word CNTEND) contain the negative logarithm of the transmissions. The pre-selected MODTRAN aerosol models are (1) no aerosol, (2) low level of aerosols [rural boundary layer with 23 km sea-level visibility and background stratospheric profiles and extinction], and (3) high level of aerosols [rural boundary layer with 5 km sea-level visibility and an extreme volcanic profile].

The file names used are (molecular formula).CNT. These files must be located in the same directory as the chemical kinetics files.

Table 8. Continuum Transmittance File for CO

```
CO     BAND TRANSITIONS FOR ISOTOPE NUMBER 1
    1-     0          2143.27 CM-1
    5   0.99849671   0.99549103   0.99398768   0.99323565   0.99248427
        0.04301865   0.33140495   0.85715795   2.21468997   13.31810570
        0.04409396   0.34464619   0.88809311   2.26152062   17.39599419
        0.04409396   4.05797625   5.64853382   5.83024502   36.60150146
CNTEND
    2-     0          4260.06 CM-1
    5   0.99849659   0.99549097   0.99398762   0.99323571   0.99248421
        0.00560784   0.09626941   0.47075126   1.24760354   6.72888994
        0.00736630   0.10396815   0.48696208   1.36213613   12.69397163
        0.00736630   7.09826565   9.48567772   8.13176441   41.72343445
CNTEND
    2-     1          2116.79 CM-1
    5   0.99849659   0.99549097   0.99398762   0.99323571   0.99248421
        0.11522912   0.82049203   1.48554504   2.81183815   15.81890678
        0.11629508   0.83339179   1.51568389   2.85765195   19.88576698
        0.11629508   4.47239161   6.18162632   6.36636448   39.02658081
CNTEND
```

6.5 Spectral Line Files

6.5.1 Modified HITRAN Line File

The augmented HITRAN [Rothman *et al.*, 1998] line file used by SAMM2 includes line parameters for 18 radiators: CO, OH, O_3, NO^+, NO, CH_4, HNO_3, N_2O, NO_2, SO_2, NH_3, four isotopes of H_2O and three isotopes of CO_2. The line file contains the spectral line information required to perform line-by-line emission calculations for each radiator. There are a total of more than 500,000 lines in the SAMM2 line file. The lines in the SAMM2 line file have been modified from the original HITRAN format to speed up the LOS spectral radiance calculation. The first modification was to separate the total energy of the lower state, E", into vibrational, E_V, and rotational, E_R, components. SAMM2 requires the separate E_V and E_R to properly scale the line strength since the vibrational and rotational temperatures can differ. Computational time is saved by storing E" and E_R rather than re-calculating them in the spectral radiance module.

The standard HITRAN line strengths have also been modified. The temperature-dependent scaling factors evaluated at the reference temperature, $T_s = 296$ K, have been removed from the strengths. This modification speeds up the spectral radiance calculation by eliminating the calculations which depend on T_s. Although the CPU savings realized by removing T_s is fairly small per line, a typical calculation uses thousands of lines and, therefore, the total savings can be significant. The line strength, SR, stored in the SAMM2 lines file database is given by:

$$SR = S(T_s)Q_v(T_s)Q_r(T_s)Q_e(T_s)exp(C_2\frac{E''}{T_s})[1 - exp(C_2\frac{W_o}{T_s})]^{-1}/I_a \ , \qquad (29)$$

where $S(T_s)$ is the standard HITRAN line strength, W_o is the transition frequency at the line center, I_a is the fractional isotopic abundance, and Q_v, Q_r, and Q_e are the vibrational, rotational, and electronic partition functions, respectively. C_2 is the second radiation constant ($C_2 = 1.43879$ cm K).

The following database parameters are used in the spectral radiance module of SAMM2:

MOL - AFGL molecular species identification label
ISO - AFGL molecular species isotope identification label
W_o - transition frequency (cm^{-1})
SR - modified line strength (cm^{-1}/molecule/cm^{-2})
GAM - Lorentz halfwidth (cm^{-1})

E" - total energy of lower state (cm^{-1})
E_R - rotational energy of lower state (cm^{-1})
ETA - coefficient of the temperature dependence of air-broadened line width
IUP - upper state vibrational label
ILOW - lower state vibrational label.

An example of the database is given in Table 9; we have included only the parameters currently used by SAMM2. This part of the line file includes lines for three isotopes of H_2O (MOL = 1), and the major isotope for O_3 (MOL = 3), CH_4 (MOL = 6), and OH (MOL = 13). Table 10 displays the eighteen (thirteen) currently supported molecular species (radiators) and their associated molecular identification labels.

The line file used by SAMM2 is written in binary format. Using a binary representation of the file saves storage space and makes the reading time shorter than if the file were stored in an ASCII format. The file is provided on the SAMM2 CD in ASCII format along with a program which converts it to binary.

Table 9. Excerpt from the SAMM2 Line Parameter Database

MOL	ISO	W_o	SR	GAM	E"	E_R	ETA	IUP	ILOW
3	1	325.023900	0.3141E-18	0.0718	959.2989	258.3679	0.5	5	2
3	1	325.043700	0.6928E-18	0.0709	903.2928	202.3618	0.5	5	2
6	1	325.089630	0.2298E-16	0.0440	2636.2571	1325.4965	0.5	2	2
1	1	325.141200	0.5015E-13	0.0687	3162.2590	1567.5090	0.5	2	2
3	1	325.164700	0.1081E-17	0.0751	841.3435	140.4125	0.5	5	2
3	1	325.183400	0.9109E-18	0.0712	865.7697	164.8387	0.5	5	2
3	1	325.218300	0.8106E-18	0.0706	880.9405	180.0095	0.5	5	2
6	1	325.273810	0.3529E-18	0.0510	2167.9641	857.2035	0.5	3	2
6	1	325.280200	0.2715E-18	0.0470	2473.1780	1162.4174	0.5	3	2
6	1	325.304880	0.7862E-19	0.0470	2473.3799	1162.6193	0.5	3	2
1	2	325.311000	0.1099E-15	0.0609	921.8950	921.8950	0.5	1	1
3	1	325.340400	0.4661E-18	0.0700	1377.0950	676.1639	0.5	5	2
6	1	325.377060	0.1288E-18	0.0360	2473.2439	1162.4833	0.5	3	2
6	1	325.449730	0.1109E-16	0.0280	3042.0859	1731.3253	0.5	2	2
3	1	325.524500	0.1016E-17	0.0746	841.2429	140.3119	0.5	5	2
1	2	325.554000	0.7320E-17	0.0502	2099.5620	2099.5620	0.5	1	1
3	1	325.568000	0.4849E-18	0.0701	1355.3521	654.4210	0.5	5	2
3	1	325.601800	0.4813E-18	0.0716	921.8952	220.9642	0.5	5	2
13	1	325.668700	0.1487E-15	0.0830	1367.6270	1241.3311	0.5	17	17
13	1	325.671300	0.2262E-13	0.0830	1367.6270	1241.3311	0.5	17	17
13	1	325.671300	0.2010E-13	0.0830	1367.6250	1241.3290	0.5	17	17
1	3	325.699000	0.2701E-16	0.0465	884.1140	884.1140	0.5	1	1
1	3	325.741000	0.8105E-16	0.0460	884.0780	884.0780	0.5	1	1
1	1	325.785400	0.1675E-12	0.0598	2398.3821	803.6321	0.5	2	2
3	1	325.792400	0.5056E-18	0.0702	1334.4430	633.5120	0.5	5	2

Table 10. SAMM2 Radiators and Identification Number

CHEMICAL SPECIES	IDENTIFICATION NUMBER	ISOTOPE NUMBER
H_2O	1	1
H_2O	1	2
H_2O	1	3
H_2O	1	4
CO_2	2	1
CO_2	2	2
CO_2	2	3
O_3	3	1
N_2O	4	1
CO	5	1
CH_4	6	1
NO	8	1
SO2	9	1
NO2	10	1
NH3	11	1
HNO3	12	1
OH	13	1
NO^+	36	1

6.5.2 LTE Line Tails File

Computational time is saved in the RT step by pre-summing the absorption from tails of multiple lines to avoid calculating them LBL (line-by-line) on the fly. This data file contains the Pade approximate coefficients that parameterize the extended line tails contributions to the 0.5 cm^{-1} spectral bins processed by the QBL RT algorithm. For each spectral bin, a band model type approach is used to calculate LTE line tail contributions from *all* molecular lines centered at least ½ Δv (= ¼ cm^{-1}) and no more than 25 cm^{-1} from the spectral bin (see Figure 9).

In early versions of MODTRAN, the line tail band model parameters were calculated at a grid of six temperatures (180K, 205K, 230K, 255K, 270K, and 305K) by summing all the contributing Lorentzian line tails integrated over the spectral bin centered at frequency v_c:

$$k^a\ (\textit{extended line tail at } v_c)\ =\ \frac{1}{\Delta v} \sum_L \int_{v_c - \frac{\Delta v}{2}}^{v_c + \frac{\Delta v}{2}} \frac{S_L\, \gamma_c\, /\, \pi}{(v' - v_L)^2 + \gamma_c^2}\, dv'$$

(30)

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More recently, MODTRAN has sub-divided the spectral interval into 4 equal sub-intervals to more accurately capture the spectral variation across the interval.

For SAMM2, the MODTRAN line tail calculation is further improved by explicitly fitting the spectral dependence to a Padé approximate:

$$k_\nu^a (\textit{extended line tail at } v_c) \;=\; \frac{k_0 + k_1\delta + k_2\delta^2}{1 + a\delta + b\delta^2} \;\;;\;\; \delta \;=\; 2\left(\frac{v - v_c}{\Delta v}\right) \quad . \quad (31)$$

This functional form works well because (1) it reduces to the exact expression if the line tail arises from a dominant or single line, (2) the linear terms model the asymmetry of the tail contributions, and (3) the quadratic terms enable the form to capture the single minimum that may arise due to competing (or identical) contributions from the two sides of the interval. For SAMM2, the Pade approximate coefficients are determined from the lines data file at a grid of 12 temperatures.

For structure calculations, the derivative of the LTE extended line tails with respect to translational temperature is required. The spectral dependence of the temperature derivatives is modeled using the same Padé approximate form as used for the line tails themselves. The explicit temperature derivatives of the Pade approximate coefficients are computed from the SAMM2 lines file data, and stored in the lines tails file as well.

6.5.3 Voigt Profile Parameters File

The Voigt line shape function is defined as

$$f_{\gamma_c,\gamma_D}\left(v' - v_L\right) = \frac{a\sqrt{\ln 2}}{\pi\gamma_D} \int_{-\infty}^{\infty} \frac{e^{-y^2}\,dy}{a^2 + \left(\varsigma - y\right)^2} \tag{32}$$

where $\varsigma \equiv \sqrt{\ln 2}\,\dfrac{v' - v_L}{\gamma_D}$ and $a \equiv \sqrt{\ln 2}\,\dfrac{\gamma_c}{\gamma_D}$

The Voigt profile data file contains the parameters describing the Voigt profile line shape, the integral under it, and its derivative, tabulated as functions of $\dfrac{\varsigma}{a}$ and a, where $\dfrac{\varsigma}{a}$ is the ratio of the displacement $\delta\omega$ from the line center to the Lorentz half width γ_c, and a is the ratio of γ_c over the Doppler half width γ_D.

The integrals $aF_{\gamma_C,\gamma_D}(n) \equiv a\int_{n\delta v}^{\infty} f_{\gamma_C,\gamma_D}(\omega)d\omega$ are required to calculate the absorption from local line

tails (see Figures 9). These are computed as functions of $\frac{\varsigma}{a}$ and a and stored in the Voigt profile data

file as the array VOIGT_AREA(I,J).

For structure calculations, desired quantities can be obtained from the Voigt functions themselves or their derivatives. The derivatives with respect to temperature of the local tail contributions require the quantities:

$$\frac{\partial F_{\gamma_C,\gamma_D}(n)}{\partial T} \equiv \frac{\partial\gamma_C}{\partial T}\frac{\partial F_{\gamma_C,\gamma_D}(n)}{\partial\gamma_C} + \frac{\partial\gamma_D}{\partial T}\frac{\partial F_{\gamma_C,\gamma_D}(n)}{\partial\gamma_D} \tag{33}$$

where:

$$\frac{\partial F_{\gamma_C,\gamma_D}(n)}{\partial\gamma_C} = \frac{S}{\pi}\frac{\sqrt{\ln 2}}{\gamma_D}\int_{-\infty}^{\infty}\frac{(\varsigma-y)e^{-y^2}dy}{a^2+(\varsigma-y)^2} \equiv \frac{SaV_I\left(\frac{\varsigma}{a},a\right)}{\gamma_C} \tag{34}$$

and

$$\frac{\partial F_{\gamma_C,\gamma_D}(n)}{\partial\gamma_D} \equiv \frac{SaV_R\left(\frac{\varsigma}{a},a\right)n\delta v}{\gamma_C\gamma_D} - \frac{SaV_I\left(\frac{\varsigma}{a},a\right)}{\gamma_D}. \tag{35}$$

The quantities V_R and V_I are respectively the real and imaginary parts of the Complex Voigt

function. $aV_R\left(\frac{\varsigma}{a},a\right)$ and $aV_I\left(\frac{\varsigma}{a},a\right)$ are tabulated as functions of $\frac{\varsigma}{a}$ and a, and stored in the Voigt

profile data file as the arrays VR(I,J) and VI(I,J). The derivatives of the Voigt profile itself are also required:

$$\frac{S}{\delta v}\int_{(n-1/2)\delta v}^{(n+1/2)\delta v}\frac{\partial}{\partial T}f_{\gamma_C,\gamma_D}(\omega)d\omega \approx S\frac{\partial}{\partial T}f_{\gamma_C,\gamma_D}(n\delta v) \equiv \mathrm{Re}\frac{\partial W(z)}{\partial T} =$$

$$\vdots \qquad \mathrm{Re}\left\{\left[\left(\frac{\partial\gamma_C}{\partial T}\right)\left(\frac{\partial z}{\partial\gamma_C}\right)+\left(\frac{\partial\gamma_D}{\partial T}\right)\left(\frac{\partial z}{\partial\gamma_D}\right)\right]\frac{\partial W(z)}{\partial z}\right\} \tag{36}$$

where $W(z), z = \varsigma + ia$, is the complex Voigt Function. The real and imaginary parts of the derivatives of the complex Voigt function, $W'(z)$, are computed and the quantities $a^2 \operatorname{Re} W'(z)$ and $a^2 \operatorname{Im} W'(z)$ are stored as functions of $\dfrac{\varsigma}{a}$ and a in the Voigt profile data file.

6.6 Model Atmosphere Files

A new capability, the SHARC/SAMM Atmosphere Generator (SAG) [Adler-Golden, 1993], for generating atmospheric files was introduced in SHARC-3. With the present version of SAMM2, a new version of SAG, SAG-2 [Shroll *et al.*,2003], is now provided. It is discussed in Subsection 7.2 below. Previous SHARC atmospheric profiles are no longer provided with the code (although atmospheres used for the included test cases are provided). However, the user still has the capability to provide a user-defined atmospheric profile. These models should include temperature and number densities for N_2, O_2, O, OH, CO_2, H_2O, NO, H, O_3, CH_4, CO, HNO_3, N_2O, NO_2, SO_2, and NH_3 as a function of altitude. The format of the user-defined atmospheric file is described below.

The model atmosphere file is contained in an 80 column, format free ASCII file. The atmosphere input file is checked for proper syntax and self-explanatory diagnostic messages are written to the SAMM2 journal file if unacceptable syntax is encountered.

The user can define a new atmosphere file by following a set of simple rules. A SAMM2 atmospheric file is structured as a series of input parameter identification lines followed by the actual input values (at least one) and an END line that denotes the end of the parameter input.

As an example, a high-latitude, summer night Atmosphere Model input file provided with SHARC is shown in Appendix E. As the various input parameters are described, it should help the user to refer to this appendix.

The following input parameter identification lines must be contained in the user-defined atmospheric model file in the order listed:

- ATMOSPHERE NAME Line
- NUMBER OF LAYER BOUNDARIES Line
- DAY-NIGHT VARIABLE AND EXOATMOSPHERIC TEMPERATURE Line
- SPECIES Line

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- ALTITUDES Line
- TEMPERATURES Line
- SPECIES DENSITIES Line.

Each input parameter identification line must start in Column 1. After the appropriate data corresponding to the identification line have been entered into the file in the next line, the line after next must contain the word END beginning in Column 1. The information required after each parameter identification line is detailed below.

The line following the ATMOSPHERE NAME line must contain its alphanumeric name. In the example, the name is NIG65N.ATM. Up to 32 non-blank characters are allowed. If the name does not match the actual file name, a warning is entered into the SAMM2.LOG file. After the END line (and following the NUMBER OF LAYER BOUNDARIES line), the number of layer boundary points should be entered. There must be at least 2 layer boundaries, and the current maximum is 103 boundaries, as in the example. To increase the maximum number of boundaries, the parameter NBYMAX defined in PARMS.H must be changed from 103 to the required value and SAMM2 must be re-compiled. Next, the DAY-NIGHT parameter and the EXOATMOSPHERIC TEMPERATURE should be defined exactly in the order stated and separated by at least one blank space. The DAY-NIGHT parameter is entered as either DAY (shown) or NIGHT. After the SPECIES line, a list of atmospheric species for which number densities are given is input. This list of species must include all molecular species desired in the model atmosphere. Sixteen such species appear in Appendix E, including O_2, N_2, O, and H, which are not SAMM2 radiators but are involved in the kinetics. The same rules apply to entering the atmospheric species as those given for the INTERPRETER (see Subsection 7.1.1). Also, each atmospheric species (excluding species identified as molecular vibrational states) listed in the chemical kinetics files (see Subsection 7.1.1) must be listed as a species in the atmosphere file. The ALTITUDES line precedes the next inputs considered, the altitudes of the layer boundaries. Any number of lines may be entered to define the layer altitudes. The altitudes must be entered in ascending order. The input units are km and are converted to cm for internal use. In the example, the altitudes come in rows of five, but this particular ordering is not necessary. The number of altitudes must match that specified earlier by the NUMBER OF LAYERS line, 103 here. Next, the kinetic temperatures and species number densities are entered in such a way as to correspond to the layer boundary altitudes. The number of entries for

the temperatures and each species number densities must equal the value of the NUMBER OF LAYERS parameter. The temperatures are input in degrees Kelvin and the number densities are input in molecules/cm^3. After the line containing the END line for the TEMPERATURE data, a line with one of the valid atmospheric species names (followed by a blank and the word DENSITIES) indicates the beginning of the atmospheric number densities input for this species. Again, the data is followed by the word END beginning in Column 1. The procedure for the atmospheric species is continued until number densities have been defined for all atmospheric species listed in the SPECIES section of the file.

6.7 Solar Irradiance Files

The solar irradiance files used by SAMM2 are those provided by MODTRAN4. There are 4 different solar databases which can be selected by the user:

- Corrected Kurucz database (NEWKUR.DAT)
- Chance database (CHKUR.DAT)
- Cebula plus Chance data (CEBCHKUR.DAT)
- Thuillier plus corrected Kurucz (THKUR.DAT)

These databases are provided for the spectral range of 50 to 50000 cm^{-1} at a 1 cm^{-1} spectral resolution. The solar irradiance is used in the computation of the solar pumping of molecular species and the solar scattering by aerosols and clouds. Linear interpolation is used to obtain the solar irradiance at an arbitrary frequency.

The user has the option of providing a user-defined solar irradiance file. An example of the database is given in Table 11, which is a portion of the NEWKUR.DAT file. The first two lines are descriptive and must be present. The subsequent lines contain one pair of frequency and solar irradiance per line. The units are wavenumbers (cm^{-1}) for frequency and W/cm2/cm^{-1} for solar irradiance, and the spectral resolution must be 1 cm^{-1}. The user must ensure that the frequency range covered in the file is appropriate for the spectral range of the radiation transport calculation, as well as the spectral range of the vibrational bands for the specified molecular radiators.

Table 11. Excerpt from one of the SAMM2 Solar Irradiance Files

FREQ (CM-1)	SOLAR IRRADIANCE (W CM-2 / CM-1)	SOLAR CONSTANT FOR THIS SET (W/M**2) = 1368.00 (PLEASE DO NOT EDIT THIS FILE)
50	7.979E-10	
51	7.979E-10	
52	7.979E-10	
.		
.		
.		
49998	2.268E-09	
49999	2.268E-09	
50000	2.268E-09	

6.8 Ground Definition (Reflectance) Files

6.8.1 Spectral Albedo File

The spectral dependence of the earth albedo (which equals one minus the emissivity) is specified in the spectral albedo file. The albedo has a value between 0 and 1. The surface reflection is assumed to be Lambertian. The spectral dependence of the albedo is stored in an ASCII database containing a single wavelength and albedo entry per line for a specific material. A default MODTRAN4 spectral albedo file (SPEC_ALB.DAT) is provided with SAMM2 (located in the atmdir/). Currently the choices of materials contained in SPEC_ALB.DAT file include snow, forest, farm, desert, ocean, cloud deck, sea ice, and four sample grass models. The user can select one of the default materials as described previously, modify the input for a default material, or add an additional material by modifying the SPEC_ALB.DAT. Alternatively, the user can create a new file with a user-supplied file name (which must be located in the atmdir/).

The spectral albedo file can be modified or a new file created by following the example provided in Table 12 (instructions for adding materials to the SPEC_ALB.DAT file are also provided within the file). The file can contain a series of comment lines, beginning with an exclamation point "!", which are ignored during input. All comments following an exclamation point are also ignored. For example, the file shown in Table 12 contains a table of contents detailing the materials included in the file. After the comments, there is a "header" line which contains a positive integer index and material name, separated by a blank space (unlike MODTRAN, the material name is ignored by SAMM2, that is, the selection of the spectral albedo input is determined solely by the integer index

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selected during the interactive session). The lines following the "header" line contain the spectral data entered as a single wavelength (in microns) and albedo pair per line, separated by one or more blank spaces. The spectral wavelength must be entered in increasing order. The spectral albedos should not be less than 0. or greater than 1. The end of the data set for a particular material is indicated by a line beginning with an "!".

A user-defined material may be added to the SPEC_ALB.DAT file by entering a "99 User-Defined Material" on the header line, followed by the wavelength-albedo pairs. This material can then be selected during an interactive session by selecting "99" in the SELECT SPECTRAL ALBEDO menu. Alternatively, the user can follow the format illustrated in Table 12 (or the SPEC_ALB.DAT file) to create a file containing user-modified values of the spectral albedo for the materials currently supported in the SPEC_ALB.DAT file, or add a material not contained in the SPEC_ALB.DAT file by identifying the material by the material index "99".

Table 12. Excerpt from the SAMM2 Spectral Albedo File (SPEC_ALB.DAT)

```
!Spectral albedo file
      .
      .
      .
!
!Table of Contents
!1 "snow cover"
!2 "forest"
      .
      .
      .
!99 "user description"
1  snow cover !(fresh)
    1.40   .48
    1.46   .05
    1.55   .05
      .
      .
      .
    5.     .02
   20.     .02
   50.     .02
!
      .
      .
```

6.8.2 Spectral BRDF File

As in MODTRAN4 [Berk *et al.*, 1999], there are seven BRDF model options. The symmetric Walthall [Walthall, 1985] and symmetric Sinusoidal-Walthall are empirical models; the Hapke [Hapke, 1981; Hapke, 1986], Rahman [Rahman *et al.*, 1993], Roujean [Roujean *et al.*, 1992], and Ross-Li [Wanner *et al.*, 1995; Wanner *et al.*, 1997; Lucht *et al.*, 1999] are all semi-empirical models; and the Pinty-Verstraete [Pinty and Verstraete, 1991] is a physical model. Generally, the BRDFs are numerically integrated to define surface albedo, directional (hemispheric) reflectivities and emissivities, and azimuth moments (required for interfacing to the DISORT multiple scattering routines); negative values of the BRDF (which can result from angular extrapolation of the measurement-based parameterizations) are replaced by 0. For the simple empirical models, an option to use analytic representations of the reflectance quantities is also provided.

1. Walthall Model

This model requires 4 parameters, P_1, P_2, P_3, and P_4 as user inputs

$$\rho(\theta_v, \theta_s, \Delta\varphi) \;=\; P_1 \;+\; P_2\,\theta_v\,\theta_s\,\cos(\Delta\varphi) \;+\; P_3\,\theta_v^2\,\theta_s^2 \;+\; P_4\,(\theta_v^2 + \theta_s^2) \tag{37}$$

where

> θ_v is the view zenith angle from the surface to the sensor (H_1);
> θ_s is the source zenith angle at the surface; and
> $\Delta\varphi$ is the view-to-source relative azimuth angle from the surface.

2. Analytic Walthall Model (not recommended)

This choice requires the same four parameters as the Walthall model. The reason for not recommending it is that here the directional and hemispheric reflectance integrals are done analytically. Therefore, one can have unphysical negative values of the integrals if P_1, P_2, and P_3 are not chosen carefully to represent physically consistent values. In the numeric integration performed in the Walthall model the negative values are set to 0.

3. Sinusoidal Walthall

This model requires 4 parameters P1', P2', P3', and P4' as user inputs.

$$\begin{aligned}
\rho(\theta_v, \theta_s, \Delta\varphi) \;=\; & P_1' \;+\; P_2'\,\sin\theta_v\,\sin\theta_s\,\cos(\Delta\varphi) \\
& +\; P_3'\,\sin^2\theta_v\,\sin^2\theta_s \;+\; P_4'\,(\sin^2\theta_v + \sin^2\theta_s)
\end{aligned} \tag{38}$$

The sinusoidal Walthall form was introduced to facilitate Monte-Carlo sampling of photon trajectories. The sinusoidal Walthall parameters can be approximated from the Walthall parameters by equating zenith integrations, term-by-term. This lead to the following relationships:

$$P_1' = P_1$$
$$P_2' = 9 \pi^2 P_2 / 64$$
$$P_3' = (\pi^2/4-1)^2 P_3$$
$$P_4' = (\pi^2/4-1) P_4$$

4. Analytic Sinusoidal Walthall (not recommended)

This choice requires the same 4 parameters as the Sinusoidal Walthall model. The reason for not recommending it is that here the directional and hemispherical reflectance integrals are done analytically. Therefore, one can have unphysical negative values of the integrals if the four parameters are not chosen carefully to represent physically consistent values. In the numeric integration performed in the Sinusoidal Walthall model the negative values are set to 0.

5. Hapke Model

This model requires 4 parameters P1, P2, P3, and P4 as user inputs.

$$\rho(\theta_v, \theta_s, \Delta\varphi) =$$

$$\frac{P_1 / 4}{\cos\theta_v + \cos\theta_s} \left\{ \left[1 + \frac{P_4 / P_1}{B(\cos\phi, P_2, P_3)} \right] P_{HG}(\cos\phi, P_2) + H(\cos\theta_v, P_1) H(\cos\theta_s, P_1) - 1 \right\} \tag{39}$$

where

$$\cos\phi = \cos\theta_v \cos\theta_s + \sin\theta_v \sin\theta_s \cos\Delta\varphi$$

$$P_{HG}(\cos\phi, g) = \frac{1 - g^2}{(1 + g^2 + 2 g \cos\phi)^{3/2}}$$

$$B(\cos\phi, g, h) = \frac{1 - g}{(1 + g)^2} \left[1 + \frac{\sqrt{(1 + \cos\phi)/(1 - \cos\phi)}}{h} \right]$$

$$H(x, \omega) = \frac{1 + 2 x}{1 + 2 x \sqrt{1 - \omega}}$$

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Parameter $P_1 = \omega$ is the average single scattering albedo of the particles making up the surface; parameter $P_2 = g$ is the Henyey-Greenstein asymmetry factor ranging from -1 (backward scattering) to $+1$ (forward scattering); parameter $P_3 = h$ controls the width of the opposition effect (hot spot); and parameter $P_4 = S_H$ controls the magnitude of the opposition effect (S_H is a measured parameter which describes the probability that light incident on a particle will leave near the directly illuminated particle surface). [Note that the atmospheric radiative transport convention for the Henyey-Greenstein variables has been adopted in these equations. The BRDF community generally represents the asymmetry factor with the symbol Θ (instead of g) and represents the scattering angle with the symbol g (instead of ϕ) – a confusing state of affairs to say the least.

6. Rahman Model

This model requires 3 parameters P_1, P_2 and P_3 as user inputs.

$$\rho(\theta_v, \theta_s, \Delta\varphi) = P_1 \, [\cos\theta_v \, \cos\theta_s \, (\cos\theta_v + \cos\theta_s)]^{P_3 - 1} \, P_{HG}(\cos\phi, P_2) \, [1 + \frac{1 - P_1}{1 + G(\theta_v, \theta_s, \Delta\varphi)}] \tag{40}$$

where

$$G(\theta_v, \theta_s, \Delta\varphi) = \sqrt{\tan^2\theta_v + \tan^2\theta_s - 2\tan\theta_v \tan\theta_s \cos\Delta\varphi}$$

Parameter $P_1 = \rho_0 \geq 0$ characterizes the reflectance of the surface cover; parameter $P_2 = g$ is the Henyey-Greenstein asymmetry factor ranging from -1 (backward scattering) to $+1$ (forward scattering); and parameter $P_3 = k$ indicates the level of anisotropy of the surface.

7. Roujean Model

This model requires 3 parameters P_1, P_2 and P_3 as user inputs.

$$\rho(\theta_v, \theta_s, \Delta\varphi) = P_1 + P_2 \, K_{geo}(\theta_v, \theta_s, \Delta\varphi) + \frac{4}{3\pi} P_3 \, K_{RT}(\theta_v, \theta_s, \Delta\varphi) \tag{41}$$

where

$$K_{geo} = \frac{(\pi - \Delta\varphi)\cos\Delta\varphi + \sin\Delta\varphi}{2\pi}\tan\theta_v\tan\theta_s - \frac{\tan\theta_v + \tan\theta_s + G(\theta_v, \theta_s, \Delta\varphi)}{\pi}$$

$$K_{RT} = \frac{(\pi/2 - \phi)\cos\phi + \sin\phi}{\cos\theta_v + \cos\theta_s} - \frac{\pi}{4}$$

Parameter $P_1 = k_{Lamb}$ is the Lambertian scattering component and equal to the bidirectional reflectance for $\theta_v = 0$ and $\theta_s = 0$. Parameter $P_2 = k_{geo}$ is the coefficient of the geometric scattering kernel K_{geo}, and parameter $P_3 = k_{vol}$ is the coefficient for the Ross Thick volume scattering kernel KRT, so called for its assumption of a dense leaf canopy.

8. Pinty-Verstraete Model

This model requires 4 parameters P_1, P_2, P_3, and P_4 as user inputs.

$$\rho(\theta_v, \theta_s, \Delta\varphi) = \frac{P_1/4}{\cos\theta_v + \kappa_v(P_3)\left(\dfrac{\cos\theta_s}{\kappa_s(P_3)}\right)} \ *$$

$$\left\{ T(\theta_v, \theta_x, \Delta\varphi, P_3, P_4)\, P_{HG}(\cos\phi, P_2) + H\left[\left(\frac{\cos\theta_v}{\kappa_v(P_3)}\right), P_1\right] H\left[\left(\frac{\cos\theta_s}{\kappa_s(P_3)}\right), P_1\right] - 1 \right\} \tag{42}$$

where

$$T(\theta_v, \theta_s, \Delta\varphi, \chi_l, r\Lambda) = 1 + \frac{1}{1 + \left(4 - \dfrac{16}{3\pi}\right)\left(\dfrac{\cos\theta_v}{\kappa_v(\chi_l)}\right)\left(\dfrac{G(\theta_v, \theta_s, \Delta\varphi)}{r\Lambda}\right)}$$

$$\kappa_x(\chi_l) = 1 - \Psi(\chi_l) + 1.754\,\Psi(\chi_l)\cos\theta_x$$

$$\Psi(\chi_l) = (1.2666 + 0.66\,\chi_l)\,\chi_l\,; \quad x = v\ or\ s$$

Parameter $P_1 = \omega$ is the average single scattering albedo of the particles making up the surface; parameter $P_2 = g$ is the Henyey-Greenstein asymmetry factor ranging from -1 (backward scattering) to $+1$ (forward scattering); parameter $P_3 = \chi_l$ is most negative (-0.4) for an erectophile canopy (mostly vertical scatterers), 0. for a canopy with a uniform distribution (equal probability for all scatterer orientations), and most positive (0.6) for a planophile canopy (mostly horizontal scatterers); and parameter $P_4 = r\Lambda$ is the product of r, the radius of the Sun flecks on the inclined scatterers, and

Λ, the scatterer area density of the canopy (expressed as the scatterer surface per unit bulk area). Note that the functions describing the orientation distribution of the scatterers for the illumination and viewing angles, κ_v and κ_s, are defined here as twice their normal value to be consistent with the definition of multiple scattering functions, $H(x, \omega)$.

9. Ross-Li Model

This model requires 5 parameters P_1, P_2, P_3, P_4, and P_5 as user inputs.

$$\rho(\theta_v, \theta_s, \Delta\varphi) \;=\; P_1 + P_2\, K_{LSR}(\theta_v, \theta_s, \Delta\varphi, P_4, P_5) + P_3\, K_{RT}(\theta_v, \theta_s, \Delta\varphi) \tag{43}$$

where

$$K_{LSR} \;=\; \frac{1 + \sec\theta_v' \sec\theta_s' + \tan\theta_v' \tan\theta_s' \cos\Delta\varphi}{2} + \left(\frac{t - \sin t \cos t}{\pi} - 1\right)(\sec\theta_v' + \sec\theta_s')$$

$$\cos^2 t \;=\; \min\left\{\left(\frac{P_4}{\sec\theta_v' + \sec\theta_s'}\right)^2 \left[G(\theta_v', \theta_s', \Delta\varphi)^2 + \left(\tan\theta_v' \tan\theta_s' \sin\Delta\varphi\right)^2\right], \; 1\right\}$$

$$\tan\theta_x' \;=\; P_5 \tan\theta_x\,; \qquad x \;=\; v \text{ or } s$$

Parameter $P_1 = k_{Lamb}$ is the Lambertian scattering component and equal to the bidirectional reflectance for $\theta_v = 0$ and $\theta_s = 0$. Parameter $P_2 = k_{geo}$ is the coefficient of the LiSparse-Reciprocal geometric scattering kernel K_{LSR}, derived for a sparse ensemble of surface objects casting shadows on a Lambertian background. Parameter $P_3 = k_{vol}$ is the coefficient for the RossThick volume scattering kernel K_{RT}, so called for its assumption of a dense leaf canopy. The two constants, dimensionless crown relative height ($P_4 = h/b$) and shape ($P_5 = b/r$) parameters have been empirically obtained and should not be interpreted too literally. The Li Sparse-Reciprocal kernel has only been validated for $h/b = 2$ and $b/r = 1$. These are the recommended constant input values for parameters P_4 and P_5.

The user can define a SAMM2 BRDF parameters file by following the format illustrated in Table 13. The file is structured as a series of comment lines, beginning with an exclamation point ('!'), followed by a line containing the number of wavelengths at which the parameters are specified, the zenith of the surface normal (which currently is always set to 0.0), and the azimuth of the surface normal (defined as 0° N, 90° E, etc.), which is not currently used. The subsequent lines contain the

wavelengths in microns (in increasing order) and the values of the BRDF parameters with one set of wavelength and parameters per line. For example, the Walthall BRDF model in Table 13 requires four parameters (P_1, P_2, P_3, and P_4) as a function of wavelength.

Table 13. Excerpt from the SAMM2 Spectral BRDF File for the Walthall Model

```
! Spectral BRDF file for the Walthall BRDF Model – Desert
!
! All lines beginning with '!' are comment lines.
! All comment lines come before data and none after it.
! No blank lines before data are permitted, unless beginning with a '!'.
!
! First line of data contains number of wavelengths, zenith of surface normal
! (now always 0.0) and azimuth of surf normal (0 N, 90 E; currently unused).
! The subsequent lines contain the wavelength (in microns) and all
! corresponding parameters.
!
! The number of parameters for each model is described in the SAMM2 manual.
!
2 0. 0.
3.99  0.4035  0.1095  0.1254  -0.0498
4.00  0.4615  0.1127  0.1305  -0.0509
```

6.9 Temperature Statistics File

SAMM2 is delivered with the original NSS [Strugala *et al.*, 1993] temperature statistics model. The NSS model, with a default set of model parameters, was generated from the analysis of in-situ measurements of the density, temperature and species concentrations. A preferred set of temperature statistics parameters, based on recent analyses of infrared MSX limb structure observations, is also provided for the NSS model. There are options available through the interactive input module which allows the user to scale the temperature variance and correlation lengths by constant multiplicative factors. This option is useful for parametric studies on the size of the temperature statistics and their effects on the radiance statistics. The user can also select the vertical and horizontal spectral indices for the temperature PSD. The model provides a covariance function, PSD description of atmospheric temperature and density fluctuations. SAMM2 expects the temperature statistics file to include the relative standard deviation and horizontal and vertical correlation lengths (km) as a function of altitude (km).

The temperature statistics file is contained in an 80 column, format free ASCII file. The input file is checked for proper syntax and self-explanatory diagnostic messages are written to the SAMM2 journal file if unacceptable syntax is encountered.

The user can define a new file by following a set of simple rules. A SAMM2 temperature statistics file is structured as a series of input parameter identification lines followed by the actual input values (at least one) and an END line that denotes the end of the parameter input.

The following input parameter identification lines must be contained in the user-defined atmospheric model file in the order listed:

- STANDARD DEVIATIONS AS FUNCTION OF ALTITUDE
- VERTICAL CORRELATION LENGTHS AS FUNCTION OF ALTITUDE
- HORIZONTAL CORRELATION LENGTHS AS FUNCTION OF ALTITUDE.

Each input parameter identification line must start in Column 1. After the appropriate data corresponding to the identification line have been entered into the file in the next line, the line after next must contain the word END beginning in Column 1. The information required after each parameter identification line consists of two columns of information. First the relative standard deviation or correlation length (km) followed by the corresponding altitude (km).

6.10 Required Correspondences Between Data Files

The data files supplied with SAMM2 are mutually consistent, supplying all the information needed for each radiator with the chosen kinetics scheme. In modifying these files to support an extended or new kinetics or set of states and transitions, the user must insure that changes are made in all the files which require change. Requirements for the individual files have been discussed above; this section points out how to keep data files consistent after modifications.

The kinetics file both establishes the kinetic scheme and constrains the effect that the states and bands files can have. A state or transition which is not called out here will not contribute to the calculation, and if added to the states or bands file it will generally result in an error, warning or caution printed to the SAMM2.LOG file. When a transition is added to the kinetics file, both the forward and the reverse processes must be added. Vibration-translation processes are excepted. The

user should remember that, unlike the case for the states and bands files, a change to the kinetics file alone does not affect SAMM2 calculations; after the change, the INTERPRETER must be used to generate the ASCII linking file. The derived linking file, not the source kinetics file, is what SAMM2 reads and uses.

The states and transitions in the states file should ideally match those in the kinetics file one to one. The bands file must then also acquire new bands corresponding to the new transitions, with each new band having all lines pertaining to that transition. Finally, the continuum file should receive the same new bands as the bands file.

It is highly recommended that any changes follow this rule of one to one correspondence, with new states and transitions/bands appearing also in the kinetics file, even with zero rate constants. SAMM2 will nonetheless run successfully for some departures from this rule. If a states-file line for a new energy is added, SAMM2 will run, with no messages commenting on the addition, and the results will be unchanged. If also, a states-file transition involving that new state is added, the run will terminate with an error message noting that the state is not in the species list of the linking file (derived from the kinetics file).

If a new transition is placed in the kinetics file but omitted from the states file, while the new state's energy is included in the states file, SAMM2 will run to completion. However, the new transition will have no impact on the output. The states-file transition line is needed before SAMM2 will include that transition.

Once a new state and one or more of its transitions have been placed correctly in the linking and states files, the bands file must be updated; a missing transition here will stop SAMM2 with an error message. The lines occurring for each new transition must be sorted into the appropriate strength bins as discussed in Subsection 6.3. As was the case for an extra energy line in the states file, an extra band in the bands file will result in a successful run with no change to the output. In this case, however, a caution will be written noting that any new energy level involved in the band does not appear in the kinetics file. If, in addition, the new states are added to the states and linking file, an error will result.

Finally, solar absorbance by the lower atmosphere is defined by the continuum transmittance files. Any change in the bands file, in either the transitions considered, or in the specific bins within a transition, must be reflected in corresponding changes in the continuum transmittance files, or SAMM2 will stop with an error, such as:

```
ERROR IN LOWIN...
    MISMATCH IN BIN NUMBER FOR THE   CO(1) - CO(0)       BAND
```

This is a message from SAMM2. The name of the continuum transmittance file is created by appending the string ".CNT" to the molecular formula. A missing continuum transmittance file will be evidenced by a FORTRAN runtime error, such as:

```
Fortran runtime error on external file "kindir/CO.CNT" (2):
    No such file or directory
```

resulting from an attempt to open the nonexistent file. The above is a message from the FORTRAN compiler; SAMM2 does not check for the existence of the file before trying to open it. The exact message would depend on the compiler used. Note, SAMM2 will attempt to use this file only if the solar zenith is between $90°$ and $108°$.

In brief, partial modifications to the SAMM2 data files may result in an apparently successful run, perhaps with warning or caution messages, which does not express the kinetic scheme the user intended. Most such modifications result in an error message and an incomplete calculation. The best policy is to make only complete changes. To do so, the user should check that a new energy is added to both the kinetics and states file, a new transition to all four files, and that the linking file has in fact been compiled from the current kinetics file.

6.11 Data File Summary

To execute SAMM2 the user must first prepare several input files. Many of these files require no modification by the user unless the user desires to change and/or supplement the database provided with SAMM2. The SAMM2 input and output files are summarized in Table 14. These files are:

- 20 Linking files (one for each molecular radiator),

- 20 States files (one for each molecular radiator),

- 17 Bands files (one for each molecular radiator, none required for auroral species),

- 17 continuum transmission files (one for each molecular radiator, none for auroral species),

- Model atmosphere profile file(s) (17 are provided),

- Model solar irradiance file (4 are provided),

- Ground definition (reflectance) file (3 are provided),

- Model temperature statistics profile file (2 are provided),

- SAMM2 HITRAN file (binary version),

- SAMM2 LTE line tails file (binary version),

- SAMM2 Voigt profile parameters file (binary version), and

- SAMM2 input file (SAMM2.INP).

Table 14. Summary of the Files Used by SAMM2.

LINKING	STATES	BANDS	CONTINUUM	INPUT	OUTPUT
CO.CKL	CO.STA	CO.BND	CO.CNT	SAMM2.INP*	SAMM2.LOG
NO.CKL	NO.STA	NO.BND	NO.CNT	SAMM96.BIN[#]	SAMM2.OUT*
O3.CKL	O3.STA	O3.BND	O3.CNT	LTETAIL.BIN[#]	SAMM2.SPC*
OH.CKL	OH.STA	OH.BND	OH.CNT	VOIGTPROFILE.BIN[#]	SAMM2.TRN*
CH4.CKL	CH4.STA	CH4.BND	CH4.CNT		SAMM2.BRD*
H2O1.CKL	H2O1.STA	H2O1.BND	H2O1.CNT		POPNEW.DAT*
H2O2.CKL	H2O2.STA	H2O2.BND	H2O2.CNT	DAY35N.ATM[%]	
H2O3.CKL	H2O3.STA	H2O3.BND	H2O3.CNT	STATS_NSS.DAT[%]	
H2O4.CKL	H2O4.STA	H2O4.BND	H2O4.CNT	NEWKUR.DAT[%]	
CO21.CKL	CO21.STA	CO21.BND	CO21.CNT	SPEC_ALB.DAT[%]	
CO22.CKL	CO22.STA	CO22.BND	CO22.CNT	WALTHALL.DAT[%]	
CO23.CKL	CO23.STA	CO23.BND	CO23.CNT		
HNO3.CKL	HNO3.STA	HNO3.BND	HNO3.CNT		

N2O.CKL	N2O.STA	N2O.BND	N2O.CNT
NH3.CKL	NH3.STA	NH3.BND	NH3.CNT
NO2.CKL	NO2.STA	NO2.BND	NO2.CNT
SO2.CKL	SO2.STA	SO2.BND	SO2.CNT
ACO2.CKL	ACO2.STA		
ANO.CKL	ANO.STA		
ANOP.CKL	ANOP.STA		

* User-supplied name.

These files must be created by the user prior to running SAMM2.

% This is one of the model atmosphere, solar, or material reflectance files supplied.

The data files required by SAMM2 are described in Subsections 6.1-6.9. Default linking files are provided with SAMM2 and only require modification if the user changes the chemical kinetics schemes. New linking files corresponding to user modified or created chemical kinetics mechanisms are generated by running the INTERPRETER and are described in Section 7. The states, bands, low-altitude continuum, model atmosphere, and solar irradiance files are provided with the code and require no modification. Material reflectance files are also provided with the code, and may require modification depending on the application. The binary SAMM2 HITRAN, line tail, and Voigt profile parameter files (see Subsection 6.5) are generated from their respective ASCII files provided with SAMM2. Forming these binary files and compiling/linking SAMM2 are described in Appendix A. Finally the SAMM2 input file, SAMM2.INP, must be available to SAMM2, or a new SAMM2.INP will be created. The input module and the SAMM2.INP files are described in Section 3.

7. AUXILIARY SAMM2 PROGRAMS

7.1 The INTERPRETER Program

The SAMM2 CHEMKIN module computes the steady-state and time-dependent number densities of vibrationally excited atmospheric species from a set of chemical kinetics/reaction mechanisms. The chemical kinetics mechanism describes molecular formation, all forms of vibrational energy transfer, and the absorption of solar and/or earthshine radiation. SAMM2's access to the chemical kinetics mechanism and associated input (that is, energy transfer or reaction rate constants) is provided by a program called the INTERPRETER, found in the FORTRAN file called interp.f. The INTERPRETER reads the chemical kinetics data base and creates an ASCII "linking" file with this information. The SAMM2 INTERPRETER is based entirely on and includes subroutines directly from the Sandia Livermore INTERPRETER code which is provided with the CHEMKIN code [Kee *et al.*, 1980]. The CHEMKIN package is described as "a general-purpose, problem-independent, transportable, FORTRAN chemical kinetics code." The SAMM2 INTERPRETER is a modified CHEMKIN interpreter from which information on elements in the periodic table and the thermodynamic data base (useful for combustion reactions, but extraneous to this application) has been removed.

Once the chemical kinetics mechanism has been formulated, the INTERPRETER provides the vehicle by which the information is transferred to the CHEMKIN module in SAMM2. The INTERPRETER reads a symbolic description of an arbitrary chemical kinetics mechanism in a manner that is just as would be written by a chemical kineticist; it then translates this information into the appropriate differential rate equations. Consider I irreversible kinetic (energy transfer or reactive) processes involving L species. Each process is expressed in the general form

$$\sum_{l=1}^{L} v(l,i) C_l \rightarrow \sum_{l=1}^{L} v'(l,i) \ C_l. \tag{44}$$

The stoichiometric coefficients of the lth species in the ith process, $v(l,i)$, are integers. C_l is the chemical symbol for the lth species; and k_i is the rate constant for the ith process. The INTERPRETER reads this symbolic description of an arbitrary chemical kinetics mechanism and

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provides the data necessary to translate the mechanism into the appropriate differential equations for the production rates of the species. The production rate for the jth species, $d[C_j]/dt$, is given by

$$\frac{d[C_j]}{dt} = \sum_{i=1}^{I} (v'(j,i) - v(j,i)) k_i \prod_{l=1}^{L} [C_l]^{v(l,i)}. \tag{45}$$

All the variables defined in Equations (44) and (45) are written into an ASCII "linking" file. Although this example is shown for irreversible processes, it should be noted that SAMM2 allows the use of reversible vibrational to translational processes. However, reversible vibrational to vibrational energy exchange processes must still be explicitly entered as irreversible reactions in the forward and reverse directions. The INTERPRETER only has to be run once for a given kinetics mechanism and data base. The "linking" file is then saved and used by SAMM2 for all subsequent calculations. Of course, if the kinetics mechanism or data base is changed, the INTERPRETER has to be rerun.

The INTERPRETER needs an ASCII input file named INTERP.INP, which contains the chemical kinetics mechanism for producing vibrationally excited states for the selected radiator. The structure for this input file is discussed below. After execution of the INTERPRETER, two output files are created: INTERP.OUT and INTERP.CKL. The file INTERP.OUT is an ASCII file and contains information from the input file. The user should check this file to ensure that the INTERPRETER was successfully executed. Any error messages created during program execution will be written to this file. The file INTERP.CKL is an ASCII file (that is, the "linking" file) which contains the chemical kinetics information required by SAMM2. This file is only created if no errors were encountered during the INTERPRETER execution.

Twelve chemical kinetics mechanism input files are currently supplied with SAMM2 for the NLTE species - CO, NO, O_3, OH, CH_4, four isotopes of H_2O, and three isotopes of CO_2. There are also five kinetics files for low-altitude species (HNO_3, N_2O, NO_2, SO_2, and NH_3) which have no chemical kinetics mechanisms specified since they are treated as LTE radiators. Finally, there are auroral kinetic files for the primary isotope of CO_2, NO^+ and NO. The input file names are summarized in Table 15. In order to create a "linking" file for one of the radiators, say CO, one would proceed as follows:

(1) copy the file CO.KIN to INTERP.INP,

(2) execute the INTERPRETER,

(3) rename INTERP.OUT to CO.OUT, and

(4) rename INTERP.CKL to CO.CKL.

The file CO.CKL would then be used as the CO "linking" file for SAMM2. This procedure must be carried out for each molecular radiator, each H_2O and CO_2 isotope being considered as a separate species. A UNIX script file, interp.run, performs these four steps for each molecular radiator automatically. This file is provided with SAMM2. The interp.run (an analogous file, Interp.bat, can be used for generating these files on a PC) file assumes that the INTERPRETER executable file is called "interp.exe".

Table 15. Files Used by the INTERPRETER.

INPUT	OUTPUT	LINKING
CO.KIN	CO.OUT	CO.CKL
NO.KIN	NO.OUT	NO.CKL
O3.KIN	O3.OUT	O3.CKL
OH.KIN	OH.OUT	OH.CKL
CH4.KIN	CH4.OUT	CH4.CKL
H2O1.KIN	H2O1.OUT	H2O1.CKL
H2O2.KIN	H2O2.OUT	H2O2.CKL
H2O3.KIN	H2O3.OUT	H2O3.CKL
H2O4.KIN	H2O4.OUT	H2O4.CKL
CO21.KIN	CO21.OUT	CO21.CKL
CO22.KIN	CO22.OUT	CO22.CKL
CO23.KIN	CO23.OUT	CO23.CKL
N2O.KIN	N2O.OUT	N2O.CKL
SO2.KIN	SO2.OUT	SO2.CKL
NO2.KIN	NO2.OUT	NO2.CKL
NH3.KIN	NH3.OUT	NH3.CKL
HNO3.KIN	HNO3.OUT	HNO3.CKL
ACO2.KIN	ACO2.OUT	ACO2.CKL
ANO.KIN	ANO.OUT	ANO.CKL
ANOP.KIN	ANOP.OUT	ANOP.CKL

7.1.1 Creating the INTERPRETER Input Files

The INTERPRETER reads the symbolic description of a chemical kinetics mechanism from the INTERP.INP file and writes the information describing the mechanism to the INTERP.CKL file for subsequent use by the CHEMKIN module. The input required by the INTERPRETER is the species

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name used in the mechanism and the mechanism itself. An example of the CO chemical kinetics mechanism input file currently used by SAMM2 is given in Table 16.

The information contained in the input file is given in an 80-column format. All input to the INTERPRETER is format free. The INTERPRETER checks each input line for proper syntax and writes self-explanatory diagnostic messages to the output file if bad syntax is encountered. If any errors are encountered, the INTERPRETER does not create the linking file. Therefore, the input must be error free before SAMM2 can be executed.

The rules for creating the INTERPRETER input file have been described in detail elsewhere [Kee *et al..*, 1980]. Subsection 7.1 reproduces this input procedure as previously described. Some changes to the information expected in the SAMM2 INTERPRETER input file are incorporated in these sections.

Table 16. SAMM2 INTERPRETER CO Kinetics Mechanism Input File

```
CO SHARC CHEMICAL KINETICS MECHANISM
SPECIES
N2 O2 O CO2 CO H2O NO O3 H OH
N2(0) N2(1)
CO(0) CO(1) CO(2) CH4
END
REACTIONS
M + CO(1) = M + CO(0)              9.90E-09      0.0    168.1    0.0
    N2/1.0/ O2/1.0/
O + CO(1) = O + CO(0)              2.82E-09      0.0     75.4    0.0
M + CO(2) = M + CO(1)              1.98E-08      0.0    168.1    0.0
    N2/1.0/ O2/1.0/
O + CO(2) = O + CO(1)              2.82E-09      0.0     75.4    0.0
O + CO(2) = O + CO(0)              2.82E-09      0.0     75.4    0.0
CO(0) + N2(1) - CO(1) + N2(0)      6.98E-13      0.0     25.6    0.0
CO(1) + N2(0) - CO(0) + N2(1)      6.98E-13      0.0     25.6   268.5
CO(1) - CO(0) + HV                30.96          0.0      0.0    0.0
CO(2) - CO(1) + HV                60.45          0.0      0.0    0.0
CO(2) - CO(0) + HV                 1.03          0.0      0.0    0.0
CO(0) + HV - CO(1)                 0.0           0.0      0.0    0.0
CO(0) + HV - CO(2)                 0.0           0.0      0.0    0.0
CO(1) + HV - CO(2)                 0.0           0.0      0.0    0.0
END
```

7.1.1.1 Title Line

The first line in the chemical kinetics mechanism input file contains the title identifying the radiator. The title is restricted to 80 characters and is used only for descriptive purposes in the INTERPRETER output file (INTERP.OUT). The title is not written to the INTERPRETER linking file.

7.1.1.2 Species Lines

Each chemical species must be identified on a Species Line (or lines). Any set of up to 15 characters can be used as a species name, which must begin with a letter. Species names of more than 15 characters may be used by simply changing a parameter value and some related format statements in the INTERPRETER. The primary purpose of the Species Lines is to identify the atmospheric species, the vibrational states included in the chemical kinetics mechanism for the selected radiating species, and finally the order in which arrays of species information are referenced in SAMM2.

The first Species Line must contain the word SPECIES starting in Column 1. It is then followed by any number of lines that identify the species. Species symbols may appear anywhere on the line, and those on the same line must be separated by blank spaces. After all the species have been given, the following line must contain the word END starting in Column 1. The rules for Species Lines are summarized in Table 17.

Table 17. Summary of the Rules for Species Lines.

1. The first (last) species Line must contain the word SPECIES (END) starting in Column 1. All other columns on this line are ignored.
2. Species names are composed of up to 10-character symbols. The names cannot begin with the characters +, -, =, a parenthesis, or a number.
3. Each species must be declared only once.
4. Each species that subsequently appears in a reaction must be declared.
5. The species declarations may appear anywhere on the lines.
6. Any number of species declarations may appear on a line. More than one line may be used.
7. Species declarations that appear on the same line must be separated by at least one blank space.
8. A species declaration that begins on one line may not continue to the next line.
9. One species declaration may end in Column 80 of one line and the next declaration may begin in Column 1 of the next line.

7.1.1.3 Reaction Mechanism Description

The reaction mechanism involves a number of chemical reactions and/or energy transfer processes involving the species named on the Species Lines. The first Reaction Line must contain the word REACTIONS starting in Column 1. The following lines contain the reaction description together with the generalized Arrhenius/Schwartz-Slawsky-Herzfeld (SSH) rate coefficients. The reaction description is made up of Reaction Lines and perhaps Auxiliary Information Lines. The last line of the reaction description must contain the word END starting in Column 1.

7.1.1.3.1 Reaction Lines

Each Reaction Line is divided into two fields. The first field contains the symbolic description of the reaction while the second contains the Arrhenius/SSH rate coefficients. Both fields are format free, and blank spaces are ignored (except within a number or a species symbol). The reaction description, given in the first field, must be composed of the species symbols, coefficients, delimiters, and special symbols as summarized below:

Species Symbols

> Each species in a reaction is described with the unique sequence of characters exactly as they appear in the Species Lines.

Coefficients

> Any species symbol may be preceded by an integer coefficient. The coefficient simply has the meaning that there are that many moles of the particular species present as either reactants or products; for example, 2OH is equivalent to OH + OH (non-integer coefficients are not allowed).

Delimiters

> +   A plus sign is the delimiter between the reactant species and between the product species.
>
> =   An equality sign is the delimiter between the reactants and products for a reversible reaction.
>
> -   A minus sign is the delimiter between the reactants and products for an irreversible reaction.

M   The symbol M stands for an arbitrary third body. Normally it would appear as both a reactant and a product. However, it has the identical meaning even if it appears only as a reactant or a product. An M anywhere in the reaction description indicates that a third body is participating in the reaction. In any reaction containing an M, species are specified to have third-body efficiencies, in which case the next line(s) must be Auxiliary Information lines (described below).

HV   The symbol HV indicates that photon radiation (hv) is present as either a reactant or a product. If an HV appears in a reaction description, the wavelength of the radiation may be specified on an Auxiliary Information Line (described later).

E   The symbol E is used to represent an electron. Electrons are treated just like any other species except that they are not composed of elements.

[An open bracket means that any following characters through the beginning of the numbers for the Arrhenius coefficients are comments on the reaction. For example, the comment may be used to give a reference to the source of the reaction and rate data.

A special case for reaction descriptions occurs if two or more species names are identical except for the last character in one of the names being a +, -, or = (for example, NO, NO+). The INTERPRETER always seeks to find the longest possible species name between delimiters (+, -, =). Therefore, the species NO may not be followed directly by a + as a delimiter since this would be confused with the species NO+. To prevent this confusion, the species NO must be separated from the delimiter + by at least one blank space (for example, the reaction NO + O + M = NO2+M must be written as NO + O + M = NO2 + M). However, NO + + E+M = NO + M may just as well be written as NO + + M + E = NO + M as long as NO + + is not a species. There is no ambiguity in the convention, and the worst that can happen if the blank is not included before the delimiter is that an error message will be written from the INTERPRETER. The blank will have to be inserted by the user, but there is no possibility of having a reaction misinterpreted by the code and proceeding with an incorrect reaction.

The second field of the reaction line is used to define the Arrhenius/SSH rate coefficients A_i, β_i, C_i, and E_i. The rate constants are assumed to have the following functional form

$$k_i = A_i T^\beta exp(C_i / T^{1/3} E_i / T) \quad . \tag{46}$$

The four numbers must appear in order: the first number being A_i, the second being β_i, the third being C_i, and the fourth being E_i. At least one blank space must separate the first number and the last symbol in the reaction or the comment. The four numbers must be separated by at least one blank space; be stated in either integer, floating point, or E format (for example, 123 or 123.0 or 12.3E1) and have units associated with them. The default units for A_i are cgs (cm, sec, K, and molecules), the exact units depending on the reaction. The factor β_i is dimensionless. The default units for the SSH parameters and activation energies are $K^{1/3}$ and K, respectively.

Table 18 is a summary of the Reaction Line rules, and examples of some reaction lines are shown in Table 16.

Table 18. Summary of the Rules for Reaction Lines

1. The first (last) Reaction line must contain the word REACTIONS (END) starting in Column 1. All other columns on this line are ignored. (The END line would follow the last Auxiliary Information Line, if one was used for the last reaction).
2. The reaction description can begin anywhere on the Line. All blank spaces, except those within species symbols and within coefficients, are ignored.
3. If some species names end with either the characters +, -, or =, and there are other species names that are identical except that they do not end in a +, -, or =, then in the reaction description the latter species names must be separated from +, -, or = delimiters by at least one blank space.
4. Each reaction description must use only one line and may not continue onto the next line.
5. Four numbers for the Arrhenius/SSH coefficients must appear on each Reaction Line, must occupy the last non-blank entries on the line, must be separated from the reaction description by at least one blank space, must be in the order (A_i, β_i, C_i, and E_i), and must be separated by at least one blank space. No blanks are allowed within the numbers themselves.
6. Comments are any characters following an open bracket and up to within one blank space of the first Arrhenius coefficient. The comments are written on the output file along with the reaction description, but otherwise ignored within the code.

7.1.1.3.2 Auxiliary Information Lines

If a reaction contains an M as third body and/or it contains an HV to denote radiation, the line or lines following that reaction line may be Auxiliary Information Lines. These lines specify

third-body efficiencies of certain species or specify radiation wavelength. Any species which acts as a third body must be declared as one of the species on the Species Lines.

The format of the line is a name (either a species name or the characters HV) followed by a number [either integer, floating point, or E format delimited by slashes(/)]. For enhanced third-body efficiencies, the name is the species name of the enhanced third body, and the number is its enhanced efficiency factor. For wavelength specification, the symbols HV are followed by the wavelength.

Any number of third-body efficiencies may be included, and each Auxiliary Information Line may contain one or more efficiency factors. If more than 6 species are to be specified as third bodies in any one reaction, some dimension statements need to be changed in the INTERPRETER. Also, the radiation wavelength may appear on a separate line, or it may be on the same line as a third-body efficiencies specification. Thus more than one Auxiliary Information Line may be used for any one reaction. Examples of auxiliary information are shown in Table 16. The above rules are summarized in Table 19.

Table 19. Summary of the Rules for Auxiliary Information Lines

1. Auxiliary Information Lines may only follow Reaction Lines that contain an M or an HV.
2. A species may have only one third-body efficiency associated with it in any one reaction.
3. Only one radiation wavelength may be declared in a reaction.
4. The order in which the enhanced third-body declarations are given is the order in which arrays of third-body information are referenced in the subroutine package. The order in which the radiation wavelength appears with respect to enhanced third-body information is unimportant.
5. Third-body (or wavelength) information may appear anywhere on the line.
6. Any number of third-body efficiencies may appear on a line. More than one line may be used.
7. Third-body declarations or radiation wavelength specifications that appear on the same line must be separated by at least one blank space.
8. A third-body (or wavelength) declaration that begins on one line may not continue on to the next line.
9. One declaration (third-body efficiency or wavelength) may end in column 80 of one line, and the next declaration may begin in Column 1 of the next line.
10. Any blank spaces between the species symbol (or HV) and the first slash are ignored, and any blanks between the slashes and the efficiency factor (or wavelength) are also ignored. However, no blank spaces are allowed within the factor (or wavelength).

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7.1.1.3.3 Reaction Mechanism Format Summary

The reaction mechanism may involve any number of chemical reactions and/or energy transfer processes involving the species named on the Species Lines. If more than eight species appear in a given reaction, some dimension statements in the INTERPRETER must be changed. In the INTERPRETER for SHARC-1, the energy transfer/reactive processes were written explicitly in the forward and/or reverse directions. In later versions, however, vibrational-to-translational energy transfer processes may be written in the forward direction (with reactants and products separated by the delimiter "=" rather than "-"). SAMM2 then computes the reverse rate constant using detailed balance. Vibrational-to-vibrational energy transfer processes must still be written explicitly in the forward and reverse direction. Processes may be three-body reactions with an arbitrary third body including the effects of enhanced third-body efficiencies, or may involve radiative relaxation and/or excitation (for example, earthshine and/or sunshine).

7.2 The SHARC/SAMM Atmosphere Generator

7.2.1 Purpose and Description

The SHARC/SAMM Atmosphere Generator (SAG) generates a SAMM-compatible input file of atmospheric species and kinetic temperature profiles [Adler-Golden, 1993]. A new version of SAG, SAG-2 [Shroll *et al.*, 2003], is provided with SAMM2. In addition to including the new MSIS model (NRLMSISE-00), SAG-2 contains new H_2O and NO climatologies. SAG-2 also provides an option to include improved correction factors to the O and H atom density profiles. It is currently implemented as a stand-alone, interactive FORTRAN program. The profiles are customized for the geophysical and geographic information input by the user. From information on the date, time, location, and geomagnetic and solar activity, SAG-2 accounts for systematic variabilities in CO_2, O_3, OH, NO, H_2O, and O atom densities, including terminator effects. For other species, SAG-2 utilizes diurnally-averaged profiles from recent databases. To facilitate use without detailed inputs, defaults are provided so that simple designations, such as day/night, season, latitude region (low, mid, or high), etc., can be specified as desired.

SAG-2 draws primarily on several existing atmosphere models. An empirical model, either MSISE-90 [Hedin, 1991] or NRLMSISE-00 [Picone *et al.*, 2001], is used for the temperature and major species profiles. It provides profiles for species including N_2, O_2, O, and H as a function of altitude, latitude, longitude, universal time (UT), local solar time (LST), daily Ap, F10.7, and F10.7A (30 day average).

The second atmosphere model used extensively in SAG-2 is a trace species NRL database [Summers *et al.*, 1992] for altitudes up to 120 km. It contains mean monthly species concentrations at 1 to 5 km increments and 10o latitude increments. SAG-2 interpolates between these values and converts to number densities using the MSISE-90 or NRLMSISE-00 total densities. This database is used for the SAMM2 species CH_4 and CO and for lower portions of the O_3 and O profiles, as well as for the additional species N_2O, NO_2 and HNO_3. SAG-2 has been designed to be compatible with the species and altitude ranges of SHARC, SAMM and MODTRAN.

The remaining profiles in SAG-2, including those for CO_2, NO, H_2O, OH, SO_2 and NH_3, are derived from a combination of standard concentrations [Anderson *et al.*, 1986] used in LOWTRAN and MODTRAN from photochemical or empirical models based on MSISE-90/NRLMSISE-00 inputs or outputs, or from some combination of these. In addition, SAG-2 now contains substantial upgrades to the H_2O and NO climatologies. For water vapor, the new climatology was developed by the UARS Reference Atmosphere Project (URAP), using data from the HALOE (HALogen Occulation Experiment) [Harries *et al.*, 1996], MLS (Microwave Limb Sounder Experiment) [Lahoz *et al.*, 1996], and SAGE II (Stratospheric Aerosol and Gas Experiment) [Chiou *et al.*, 1992] experiments. The Student Nitric Oxide Explorer (SNOE) database [http://lasp.colorado.edu/snoe/] has been introduced to provide nitric oxide profiles between 97 km and 150 km. The database consists of measurements of nitric oxide density in the thermosphere for the period March 11, 1998 to September 30, 2000.

The transition between the day and night profiles is handled using a simple empirical model that approximates the terminator behavior in the time-dependent calculations of Rodrigo *et al.* [1991], which were performed for mid-latitude equinox conditions above 60 km. The transition is made by linearly interpolating over a 5° range of solar zenith angle (SZA) computed for LST-0.075 hr; the 0.075 hr (4.5 min) difference accounts for the approximate photochemical lag time. The midpoint of

the interpolation region is taken to vary linearly with altitude at the rate of 0.12° per km. Based on a comparison with the calculations of Rodrigo *et al.*, this representation of the terminator location and width should be accurate to within around 1° in SZA in the 70-100 km altitude region.

7.2.2 Use and Operation

7.2.2.1 Menus

A main menu and two sub-menus are provided; they are largely self-explanatory. In the main menu, the user responds by typing an integer. The main menu reappears or a sub-menu appears following the user's response. For a detailed example of using the SAG-2 menu system, see the SAG-2 users' manual [Shroll *et al.*, 2003].

When SAG-2 is run, the variables saved from the previous run (in file "drivstor.dat") are loaded into the menus. New parameter values are entered using the two sub-menus. The Parameter Menu is used to enter numerical values, such as would pertain to a specific experimental measurement. Upon return to the main menu, a complete listing of the current parameters is given. The Default Menu is used for entering generic values. For example, the generic value of 35° latitude is entered when the latitude default designation "m" (mid-latitude) is entered. An "m" will then appear as the default value in the menu listing. If no default value is currently in use, none will appear in the listing. To display the numerical value corresponding to a default selection, enter the Parameter Menu. The SAG-2 parameter menu contains new options for using the NRLMSISE-00 empirical model in place of MSISE-90, including the URAP or SNOE databases, and improved corrections to the O atom and H atom profiles. The latitude may be entered in either geocentric or geodetic coordinates. SAG-2 uses geodetic coordinates in its calculations.

One can re-enter any parameter or menu any number of times. By using both sub-menus, any combination of default parameters and directly entered parameters can be chosen.

Certain parameters in the Parameter Menu are mutually dependent. For example, UT and LST are mutually dependent for a given longitude. After specifying the longitude, either UT or LST should be entered; the program will then automatically update the other parameter. The solar zenith angle (SZA) is also a dependent variable, being a function of the longitude, latitude, Julian day, and

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either LST or UT. The program automatically calculates and updates SZA when any of those parameters are changed. SZA can also be directly entered, in which case the longitude is recomputed from the other variables.

7.2.2.2 Altitude List and SAMM Species Option

The list of desired altitudes and the choice of SHARC or SAMM/MODTRAN species are specified in the Default Menu. Default lists exist for SAMM, SHARC, and MODTRAN. Alternatively, a custom altitude list can be input by the user from file "drivht.dat". Line 1 contains an integer argument, 0 for outputting SHARC species only or, 1 for outputting all SAMM/MODTRAN species. The number of altitudes appears on line 2. Up to 200 altitudes from 0 to 300 km are allowed. The altitude list starts on line 3; the FORTRAN general input format is used, so that either integer or floating point numbers may be entered.

7.2.2.3 List of Files

The files comprising SAG-2 as supplied with SAMM2 are as follows:

FORTRAN Source files:	afterp.f	deceqt.f	devcbd.f	dncalc.f
	dno.f	dread.f	dri.f	dump.f
	geolat.f	interp.f	ohcalc.f	outp.f
	pozone.f	sag.f	setdri.f	sintrp.f
	solzen.f	mthdmth.f	doy.f	sun.f
	tdep.f	test.f	vp.f	zenfun.f
	zenfun.f	nrlmsise00.f	modsag.f	msise90.f
	julday.f	driver.f	readinputfile.f	

4 input files:	drivstor.dat (updated by SAG-2)
	drivht.sha
	drivht.sam
	drivht.mod

10 NRL data files in subdirectory NRLDAT:			
	CH4.NRL	CO.NRL	H2O.NRL
	HNO3.NRL	N2O.NRL	NO2.NRL
	O3D.NRL	O3R.NRL	OAT.NRL
	TEMP.NRL		

1 URAP data file in subdirectory UARSDAT: H2O.DAT

1 SNOE data file in subdirectory SNOE: SNOE.DAT

Total files = 47.

7.3 The DEGRAD Program

The DEGRAD program is used to degrade the spectral resolution of the SAMM2 spectral radiance and/or transmittance data. DEGRAD is an internal SSI code delivered as a courtesy to the user. DEGRAD accepts as input the SAMM2 spectral radiance and spectral transmittance files, and enables the user to pass any of a variety of filter functions over the data. The program interactively prompts the user for all required inputs using a menu driven system. Default inputs are stored in a DEGRAD.INP file; if no such file exists, one is created when the program is executed.

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APPENDIX A
IMPLEMENTATION INSTRUCTIONS

SAMM2 is furnished with the FORTRAN source code, input data sets, and eleven test cases. The code calculates the spectral radiance and transmission from CO_2, H_2O, NO^+, NO, O_3, OH, CO, CH_4, HNO_3, N_2O, NO_2, SO_2, and NH_3 in the 250 to 5000 cm^{-1} frequency range for arbitrary geometries from 0 to 300 km. For OH, the frequency range is extended to 10000 cm^{-1} to include the spectral radiance from the $OH(\Delta v=2)$ transitions near 7000 cm^{-1}.

The CHEMKIN interpreter has one FORTRAN file. Six additional FORTRAN files contain the ASCII to binary and binary to ASCII lines files conversion programs. A spectral degrading FORTRAN routine is also included

The rest consists of 17 model atmosphere files, two temperature statistics files, four solar irradiance files, three surface reflectance files, 74 data files for the seventeen current ambient molecular radiators and the three auroral radiators, 20 interpreter output files, three ASCII line files, and input and output files for the eleven SAMM2 test cases.

The files are:

SAMM2 SOURCE CODE (directory *source*)

See Appendix C for the entire list of FORTRAN routines These are *.f files which are included in directory *source*, i.e., source/*.f.

SUPPORTING SOURCE CODES

1	kindir/interp.f	CHEMKIN Interpreter program	FORTRAN
2	lines/CONVERT/ binary_lines.f	Program to convert line data base from ASCII to binary	FORTRAN
3	lines/ CONVERT/ ascii_lines.f	Program to convert line data base from binary to ASCII	FORTRAN
4	lines/ CONVERT/ binary_tails.f	Program to convert extended line tails data base from ASCII to binary	FORTRAN
5	lines/ CONVERT/ ascii_tails.f	Program to convert extended line tails data base from binary to ASCII	FORTRAN

6	lines/ CONVERT/ binary_ voigtprofile.f	Program to convert Voigt line shape parameters data base from ASCII to binary	FORTRAN
7	lines/ CONVERT/ ascii_voigtprofile.f	Program to convert Voigt line shape parameters data base from binary to ASCII	FORTRAN
8	filtdir/degrad.f	Slit function routine	FORTRAN

MODEL ATMOSPHERES (directory *atmdir*)

1	NIG65N.ATM	High Latitude Summer Day	DATA
2	NIG35N.ATM	Mid Latitude Summer Night	DATA
3	DAY35N.ATM	Mid Latitude Summer Day	DATA
4	T4Z102.ATM	High Latitude Terminator	DATA
5	T4Z101.ATM	High Latitude Terminator	DATA
6	T4Z099.ATM	High Latitude Terminator	DATA
7	T4Z097.ATM	High Latitude Terminator	DATA
8	T4Z095.ATM	High Latitude Terminator	DATA
9	T4Z093.ATM	High Latitude Terminator	DATA
10	T4Z091.ATM	High Latitude Terminator	DATA
11	T5Z108.ATM	High Latitude Terminator	DATA
12	T5Z105.ATM	High Latitude Terminator	DATA
13	T5Z102.ATM	High Latitude Terminator	DATA
14	T5Z099.ATM	High Latitude Terminator	DATA
15	T5Z097.ATM	High Latitude Terminator	DATA
16	T5Z094.ATM	High Latitude Terminator	DATA
17	T5Z091.ATM	High Latitude Terminator	DATA

TEMPERATURE STATISTICS FILES (directory *atmdir*)

1	STATS_NSS.DAT	NSS Temperature Statistics	DATA
2	STATS_MSX.DAT	MSX Temperature Statistics	DATA

SOLAR IRRADIANCE FILES (directory *atmdir*)

1	NEWKUR.DAT	Corrected Kurucz Solar Database	DATA

2	CHKUR.DAT	Chance Solar Database	DATA
3	CEBCHKUR.DAT	Cebula-Chance Solar Database	DATA
4	THKUR.DAT	Thuillier-Corrected Kurucz Solar Database	DATA

SURFACE REFLECTANCE FILES (directory *atmdir*)

1	SPEC_ALB.DAT	Spectral Albedo Material File	DATA
2	WALTHALL.DAT	Spectral Walthall BRDF File for Desert	DATA
3	WALTHALL_A.DAT	Spectral Analytical Walthall BRDF File for Vegetation	DATA

SPECIES DATA FILES (directory *kindir*)

1	CH4.BND	CH4 Band Information file	DATA
2	CH4.KIN	CH4 Kinetics file	DATA
3	CH4.STA	CH4 Transitions and state file	DATA
4	CH4.CNT	CH4 Continuum file	DATA
5	CO.BND	CO Band Information file	DATA
6	CO.KIN	CO Kinetics file	DATA
7	CO.STA	CO Transitions and state file	DATA
8	CO.CNT	CO Continuum file	DATA
9	CO21.BND	CO2 Band Information file for 1st isotope	DATA
10	CO21.KIN	CO2 Kinetics file for 1st isotope	DATA
11	CO21.STA	CO2 Transitions and state file for 1st isotope	DATA
12	CO21.CNT	CO2 Continuum file for 1st isotope	DATA
13	CO22.BND	CO2 Band Information file for 2nd isotope	DATA
14	CO22.KIN	CO2 Kinetics file for 2nd isotope	DATA
15	CO22.STA	CO2 Transitions and state file 2nd isotope	DATA
16	CO22.CNT	CO2 Continuum file for 2nd isotope	DATA
17	CO23.BND	CO2 Band Information file for 3rd isotope	DATA
18	CO23.KIN	CO2 Kinetics file for 3rd isotope	DATA
19	CO23.STA	CO2 Transitions and state file for 3rd isotope	DATA
20	CO23.CNT	CO2 Continuum file for 3rd isotope	DATA
21	H2O1.BND	H2O Band Information file for 1st isotope	DATA
22	H2O1.KIN	H2O Kinetics file for 1st isotope	DATA

23 H2O1.STA	H2O Transitions and state file for 1st isotope	DATA
24 H2O1.CNT	H2O Continuum file for 1st Isotope	DATA
25 H2O2.BND	H2O Band Information file for 2nd Isotope	DATA
26 H2O2.KIN	H2O Kinetics file for 2nd Isotope	DATA
27 H2O2.STA	H2O Transitions and state file for 2nd Isotope	DATA
28 H2O2.CNT	H2O Continuum file for 2nd Isotope	DATA
29 H2O3.BND	H2O Band Information file for 3rd Isotope	DATA
30 H2O3.KIN	H2O Kinetics file for 3rd Isotope	DATA
31 H2O3.STA	H2O Transitions and state file for 3rd Isotope	DATA
32 H2O3.CNT	H2O Continuum file for 3rd Isotope	DATA
33 H2O4.BND	H2O Band Information file for 4th Isotope	DATA
34 H2O4.KIN	H2O Kinetics file for 4th Isotope	DATA
35 H2O4.STA	H2O Transitions and state file for 4th Isotope	DATA
36 H2O4.CNT	H2O Continuum file for 4th Isotope	DATA
37 HNO3.BND	HNO3 Band Information file	DATA
38 HNO3.KIN	HNO3 Kinetics file	DATA
39 HNO3.STA	HNO3 Transitions and state file	DATA
40 HNO3.CNT	HNO3 Continuum file	DATA
41 N2O.BND	N2O Band Information file	DATA
42 N2O.KIN	N2O Kinetics file	DATA
43 N2O.STA	N2O Transitions and state file	DATA
44 N2O.CNT	N2O Continuum file	DATA
45 NH3.BND	NH3 Band Information file	DATA
46 NH3.KIN	NH3 Kinetics file	DATA
47 NH3.STA	NH3 Transitions and state file	DATA
48 NH3.CNT	NH3 Continuum file	DATA
49 NO.BND	NO Band Information file	DATA
50 NO.KIN	NO Kinetics file	DATA
51 NO.STA	NO Transitions and state file	DATA
52 NO.CNT	NO Continuum file	DATA
43 NO2.BND	NO2 Band Information file	DATA
54 NO2.KIN	NO2 Kinetics file	DATA
55 NO2.STA	NO2 Transitions and state file	DATA
56 NO2.CNT	NO2 Continuum file	DATA
57 O3.BND	O3 Band Information file	DATA

58 O3.KIN	O3 Kinetics file	DATA
59 O3.STA	O3 Transitions and state file	DATA
60 O3.CNT	O3 Continuum file	DATA
61 OH.BND	OH Band Information file	DATA
62 OH.KIN	OH Kinetics file	DATA
63 OH.STA	OH Transitions and state file	DATA
64 OH.CNT	OH Continuum file	DATA
65 SO2.BND	SO2 Band Information file	DATA
66 SO2.KIN	SO2 Kinetics file	DATA
67 SO2.STA	SO2 Transitions and state file	DATA
68 SO2.CNT	SO2 Continuum file	DATA
69 ACO2.KIN	CO2 Auroral Kinetics file for 1st isotope	DATA
70 ACO2.STA	CO2 Auroral Transitions and state file for 1st isotope	DATA
71 ANO.KIN	NO Auroral Kinetics file	DATA
72 ANO.STA	NO Auroral Transitions and state file	DATA
73 ANOP.KIN	NO+ Auroral Kinetics file	DATA
74 ANOP.STA	NO+ Auroral Transitions and state file	DATA

INTERPRETER OUTPUT (directory *kindir*)

1 CH4.OUT	CH4 output	DATA
2 CO.OUT	CO output	DATA
3 CO21.OUT	CO2 output for 1st isotope	DATA
4 CO22.OUT	CO2 output for 2nd isotope	DATA
5 CO23.OUT	CO2 output for 3rd isotope	DATA
6 H2O1.OUT	H2O output for 1st isotope	DATA
7 H2O2.OUT	H2O output for 2nd isotope	DATA
8 H2O3.OUT	H2O output for 3rd isotope	DATA
9 H2O4.OUT	H2O output for 4th isotope	DATA
10 HNO3.OUT	HNO3 output	DATA
11 N2O.OUT	N2O output	DATA
12 NH3.OUT	NH3 output	DATA
13 NO.OUT	NO output	DATA
14 NO2.OUT	NO2 output	DATA
15 O3.OUT	O3 output	DATA

16	OH.OUT	OH output	DATA
17	SO2.OUT	SO2 output	DATA
18	ACO2.OUT	CO2 Auroral output	DATA
19	ANO.OUT	NO Auroral output	DATA
20	ANOP.OUT	NO+ Auroral output	DATA

LINE DATA FILES (directory *lines/CONVERT*)

1	SAMM96.ASC	ASCII line parameter file	DATA
2	LTETAIL.ASC	ASCII extended line tail parameter file	DATA
3	VOIGTDATA.ASC	ASCII Voigt line shape parameter file	DATA

The input files for each of the eleven test cases are found in directory *inpdir*. The same input files are also found in directory *verification* (see Appendix D), together with a comprehensive set of output files corresponding to each of the eleven test cases, including plots of comparative results to SAMM1 and MODTRAN, as well as output results from those codes. The files are:

FIRST TEST CASE (directory *verification/TEST_CASE_1/*)

SAMM2OUT/TEST1.BRD	SAMM2 Band radiance file	DATA
SAMM2OUT/TEST1.LOG	SAMM2 Journal file	DATA
SAMM2OUT/TEST1.OUT	SAMM2 General output file	DATA
SAMM2OUT/TEST1.SPC	SAMM2 Spectral radiance file	DATA
SAMM2OUT/TEST1.TRN	SAMM2 Transmission file	DATA
SAMM2INP/TEST1.INP	SAMM2 Input file	DATA
SAMM1OUT/TEST1.OUT	SAMM1 General output file	DATA
SAMM1OUT/TEST1.RAD	SAMM1 Band radiance file	DATA
SAMM1OUT/TEST1.SPC	SAMM1 Spectral radiance file	DATA
SAMM1OUT/TEST1.TRN	SAMM1 Transmission file	DATA
SAMM1INP/TEST1.INP	SAMM1 Input file	DATA
PLOTS/samm1_vs_samm2.png	Comparative plot	PLOT
PLOTS/samm1_vs_samm2_ext.png	Comparative plot	PLOT
NOTES/notes_tc1.txt	Comment	TEXT
ATMDIR/MIDLAT.NIG	Atmospheric file	DATA
ATMDIR/STATS_MSX.DAT	Temperature statistics file	DATA

SECOND TEST CASE (directory *verification/TEST_CASE_2/*)

SAMM2OUT/TEST2.BRD	SAMM2 Band radiance file	DATA
SAMM2OUT/TEST2.LOG	SAMM2 Journal file	DATA
SAMM2OUT/TEST2.OUT	SAMM2 General output file	DATA
SAMM2OUT/TEST2.SPC	SAMM2 Spectral radiance file	DATA
SAMM2OUT/TEST2.TRN	SAMM2 Transmission file	DATA
SAMM2INP/TEST2.INP	SAMM2 Input file	DATA
SAMM1OUT/TEST2.OUT	SAMM1 General output file	DATA
SAMM1OUT/TEST1.RAD	SAMM1 Band radiance file	DATA
SAMM1OUT/TEST2.SPC	SAMM1 Spectral radiance file	DATA
SAMM1OUT/TEST2.TRN	SAMM1 Transmission file	DATA
SAMM1INP/TEST2.INP	SAMM1 Input file	DATA
PLOTS/samm1_vs_samm2.png	Comparative plot	PLOT
PLOTS/samm1_vs_samm2_ext.png	Comparative plot	PLOT
NOTES/notes_tc2.txt	Comment	TEXT
ATMDIR/MIDLAT.NIG	Atmospheric file	DATA

THIRD TEST CASE (directory *verification/TEST_CASE_3/*)

SAMM2OUT/TEST3.BRD	SAMM2 Band radiance file	DATA
SAMM2OUT/TEST3.LOG	SAMM2 Journal file	DATA
SAMM2OUT/TEST3.OUT	SAMM2 General output file	DATA
SAMM2OUT/TEST3.SPC	SAMM2 Spectral radiance file	DATA
SAMM2OUT/TEST3.TRN	SAMM2 Transmission file	DATA
SAMM2OUT/TEST3_DEG.SPC	SAMM2 Degraded Spectral file	DATA
SAMM2INP/TEST3.INP	SAMM2 Input file	DATA
SAMM1OUT/TEST3.OUT	SAMM1 General output file	DATA
SAMM1OUT/TEST3.RAD	SAMM1 Band radiance file	DATA
SAMM1OUT/TEST3.SPC	SAMM1 Spectral radiance file	DATA
SAMM1OUT/TEST3.TRN	SAMM1 Transmission file	DATA
SAMM1INP/TEST3.INP	SAMM1 Input file	DATA
PLOTS/samm1_vs_samm2.png	Comparative plot	PLOT
PLOTS/samm1_vs_samm2_deg.png	Comparative plot	PLOT
PLOTS/samm1_vs_samm2_deg_ext.png	Comparative plot	PLOT

PLOTS/samm1_vs_samm2_ext1.png	Comparative plot	PLOT
PLOTS/samm1_vs_samm2_ext2.png	Comparative plot	PLOT
NOTES/notes_tc3.txt	Comment	TEXT
ATMDIR/MIDLAT.NIG	Atmospheric file	DATA

FOURTH TEST CASE (directory *verification/TEST_CASE_4/*)

SAMM2OUT/TEST4.BRD	SAMM2 Band radiance file	DATA
SAMM2OUT/TEST4.LOG	SAMM2 Journal file	DATA
SAMM2OUT/TEST4.OUT	SAMM2 General output file	DATA
SAMM2OUT/TEST4.SPC	SAMM2 Spectral radiance file	DATA
SAMM2OUT/TEST4.TRN	SAMM2 Transmission file	DATA
SAMM2INP/TEST4.INP	SAMM2 Input file	DATA
SAMM1OUT/TEST4.OUT	SAMM2 General output file	DATA
SAMM1OUT/TEST4.RAD	SAMM1 Band radiance file	DATA
SAMM1OUT/TEST4.SPC	SAMM1 Spectral radiance file	DATA
SAMM1OUT/TEST4.TRN	SAMM1 Transmission file	DATA
SAMM1INP/TEST4.INP	SAMM1 Input file	DATA
PLOTS/samm1_vs_samm2.png	Comparative plot	PLOT
NOTES/notes_tc4.txt	Comment	TEXT
ATMDIR/T4Z091.ATM	Atmospheric file	DATA
ATMDIR/T4Z093.ATM	Atmospheric file	DATA
ATMDIR/T4Z095.ATM	Atmospheric file	DATA
ATMDIR/T4Z097.ATM	Atmospheric file	DATA
ATMDIR/T4Z099.ATM	Atmospheric file	DATA
ATMDIR/T4Z101.ATM	Atmospheric file	DATA
ATMDIR/T4Z102.ATM	Atmospheric file	DATA

FIFTH TEST CASE (directory *verification/TEST_CASE_5/*)

SHARC4OUT/TEST5.OUT	SHARC4 General output file	DATA
SHARC4OUT/TEST5.SPC	SHARC4 Spectral radiance file	DATA
SHARC4OUT/TEST5.TRN	SHARC4 Transmission file	DATA
SHARC4INP/TEST5.INP	SHARC4 Input file	DATA
SHARC4ATM/T5Z91.ATM	Atmospheric file	DATA
SHARC4ATM/T5Z94.ATM	Atmospheric file	DATA
SHARC4ATM/T5Z97.ATM	Atmospheric file	DATA
SHARC4ATM/T5Z99.ATM	Atmospheric file	DATA
SHARC4ATM/T5Z102.ATM	Atmospheric file	DATA
SHARC4ATM/T5Z105.ATM	Atmospheric file	DATA
SHARC4ATM/T5Z108.ATM	Atmospheric file	DATA
SAMM2OUT/TEST5.BRD	SAMM2 Band radiance file	DATA
SAMM2OUT/TEST5.LOG	SAMM2 Journal file	DATA
SAMM2OUT/TEST5.OUT	SAMM2 General output file	DATA
SAMM2OUT/TEST5.SPC	SAMM2 Spectral radiance file	DATA
SAMM2OUT/TEST5.TRN	SAMM2 Transmission file	DATA
SAMM2INP/TEST5.INP	SAMM2 Input file	DATA
SAMM2ATM/T5Z091.ATM	Atmospheric file	DATA
SAMM2ATM/T5Z094.ATM	Atmospheric file	DATA
SAMM2ATM/T5Z097.ATM	Atmospheric file	DATA
SAMM2ATM/T5Z099.ATM	Atmospheric file	DATA
SAMM2ATM/T5Z102.ATM	Atmospheric file	DATA
SAMM2ATM/T5Z105.ATM	Atmospheric file	DATA
SAMM2ATM/T5Z108.ATM	Atmospheric file	DATA
PLOTS/sharc4_vs_samm2.png	Comparative plot	PLOT

NOTES/notes_tc5.doc	Comment	TEXT

SIXTH TEST CASE (directory *verification/TEST_CASE_6/*)

SHARC4OUT/TEST6.2D	SHARC4 2D file for the scene generator	DATA
SHARC4OUT/TEST6.3D	SHARC4 3D file for the scene generator	DATA
SHARC4OUT/TEST6.OUT	SHARC4 General output file	DATA
SHARC4OUT/TEST6.SPC	SHARC4 Spectral radiance file	DATA
SHARC4OUT/TEST6.TRN	SHARC4 Transmission file	DATA
SHARC4INP/TEST6.INP	SHARC4 Input file	DATA
SHARC4ATM/DAY35N.ATM	Atmospheric file	DATA
SHARC4ATM/STATS_SEARS.DAT	Temperature statistics file	DATA
SAMM2OUT/TEST6.2D	SAMM2 2D file for the scene generator	DATA
SAMM2OUT/TEST6.3D	SAMM2 3D file for the scene generator	DATA
SAMM2OUT/TEST6.BES	Bessel Approximation to Covariance	DATA
SAMM2OUT/TEST6.BRD	SAMM2 Band radiance file	DATA
SAMM2OUT/TEST6.COVA	Radiance Covariance vs Lag Angle	DATA
SAMM2OUT/TEST6.COVD	Radiance Covariance vs Lag Distance	DATA
SAMM2OUT/TEST6.LOG	SAMM2 Journal file	DATA
SAMM2OUT/TEST6.OUT	SAMM2 General output file	DATA
SAMM2OUT/TEST6.SPC	SAMM2 Spectral radiance file	DATA
SAMM2OUT/TEST6.TRN	SAMM2 Transmission file	DATA
SAMM2OUT/TEST6.VDIS	SAMM2 Variance Distribution file	DATA
SAMM2INP/TEST6.INP	SAMM2 Input file	DATA
SAMM2ATM/DAY35N.ATM	Atmospheric file	DATA
SAMM2ATM/STATS_SEARS.DAT	Temperature statistics file	DATA
NOTES/notes_tc6.txt	Comment	TEXT

SEVENTH TEST CASE (directory *verification/TEST_CASE_7/*)

SHARC4OUT/TEST7.2D	SHARC4 2D file for the scene generator	DATA
SHARC4OUT/TEST7.3D	SHARC4 3D file for the scene generator	DATA
SHARC4OUT/TEST7.OUT	SHARC4 General output file	DATA
SHARC4OUT/TEST7.SPC	SHARC4 Spectral radiance file	DATA
SHARC4OUT/TEST7.TRN	SHARC4 Transmission file	DATA
SHARC4INP/TEST7.INP	SHARC4 Input file	DATA
SHARC4ATM/DAY35N.ATM	Atmospheric file	DATA
SHARC4ATM/STATS_SEARS.DAT	Temperature statistics file	DATA
SAMM2OUT/TEST7.2D	SAMM2 2D file for the scene generator	DATA
SAMM2OUT/TEST7.3D	SAMM2 3D file for the scene generator	DATA
SAMM2OUT/TEST7.BES	Bessel Approximation to Covariance	DATA
SAMM2OUT/TEST7.BRD	SAMM2 Band radiance file	DATA
SAMM2OUT/TEST7.COVA	Radiance Covariance vs Lag Angle	DATA
SAMM2OUT/TEST7.COVD	Radiance Covariance vs Lag Distance	DATA
SAMM2OUT/TEST7.LOG	SAMM2 Journal file	DATA
SAMM2OUT/TEST7.OUT	SAMM2 General output file	DATA
SAMM2OUT/TEST7.SPC	SAMM2 Spectral radiance file	DATA
SAMM2OUT/TEST7.TRN	SAMM2 Transmission file	DATA
SAMM2OUT/TEST7.VDIS	SAMM2 Variance Distribution file	DATA
SAMM2INP/TEST7.INP	SAMM2 Input file	DATA
SAMM2ATM/DAY35N.ATM	Atmospheric file	DATA
SAMM2ATM/STATS_SEARS.DAT	Temperature statistics file	DATA
NOTES/notes_tc7.txt	Comment	TEXT

EIGHTH TEST CASE (directory *verification/TEST_CASE_8/*)

SHARC4OUT/TEST8.2D	SHARC4 2D file for the scene generator	DATA
SHARC4OUT/TEST8.3D	SHARC4 3D file for the scene generator	DATA
SHARC4OUT/TEST8.OUT	SHARC4 General output file	DATA
SHARC4OUT/TEST8.SPC	SHARC4 Spectral radiance file	DATA
SHARC4OUT/TEST8.TRN	SHARC4 Transmission file	DATA
SHARC4INP/TEST8.INP	SHARC4 Input file	DATA
SHARC4ATM/DAY35N.ATM	Atmospheric file	DATA
SHARC4ATM/STATS_SEARS.DAT	Temperature statistics file	DATA
SAMM2OUT/TEST8.2D	SAMM2 2D file for the scene generator	DATA
SAMM2OUT/TEST8.3D	SAMM2 3D file for the scene generator	DATA
SAMM2OUT/TEST8.BRD	SAMM2 Band radiance file	DATA
SAMM2OUT/TEST8.LOG	SAMM2 Journal file	DATA
SAMM2OUT/TEST8.OUT	SAMM2 General output file	DATA
SAMM2OUT/TEST8.SPC	SAMM2 Spectral radiance file	DATA
SAMM2OUT/TEST8.TRN	SAMM2 Transmission file	DATA
SAMM2INP/TEST8.INP	SAMM2 Input file	DATA
SAMM2ATM/DAY35N.ATM	Atmospheric file	DATA
SAMM2ATM/STATS_SEARS.DAT	Temperature statistics file	DATA
PLOTS/sharc41_vs_samm2_50km.	Comparative plot	PLOT
PLOTS/sharc41_vs_samm2_70km.	Comparative plot	PLOT
PLOTS/sharc41_vs_samm2_90km.	Comparative plot	PLOT
NOTES/notes_tc8.doc	Comment	TEXT

NINTH TEST CASE (directory *verification/TEST_CASE_9/*)

SAMM2OUT/TEST9.BRD	SAMM2 Band radiance file	DATA

SAMM2OUT/TEST9.LOG	SAMM2 Journal file	DATA
SAMM2OUT/TEST9.OUT	SAMM2 General output file	DATA
SAMM2OUT/TEST9.SPC	SAMM2 Spectral radiance file	DATA
SAMM2OUT/TEST9.TRN	SAMM2 Transmission file	DATA
SAMM2INP/TEST9.INP	SAMM2 Input file	DATA
SAMM2ATM/DAY35N.ATM	Atmospheric file	DATA
PLOTS/modtran4_vs_samm2.png	Comparative plot	PLOT
NOTES/notes_tc9.doc	Comment	TEXT
MODTRAN4OUT/TEST9.plt	MODTRAN Radiance	DATA
MODTRAN4OUT/TEST9.tp6	MODTRAN Tape 6 Output	DATA
MODTRAN4INP/TEST9.tp5	MODTRAN Tape 5 input	DATA

TENTH TEST CASE (directory *verification/TEST_CASE_10/*)

SAMM2OUT/TEST10.BRD	SAMM2 Band radiance file	DATA
SAMM2OUT/TEST10.LOG	SAMM2 Journal file	DATA
SAMM2OUT/TEST10.OUT	SAMM2 General output file	DATA
SAMM2OUT/TEST10.SPC	SAMM2 Spectral radiance file	DATA
SAMM2OUT/TEST10.TRN	SAMM2 Transmission file	DATA
SAMM2INP/TEST10.INP	SAMM2 Input file	DATA
SAMM2ATM/DAY35N.ATM	Atmospheric file	DATA
PLOTS/modtran4_vs_samm2.png	Comparative plot	PLOT
NOTES/notes_tc10.doc	Comment	TEXT
MODTRAN4OUT/TEST10.plt	MODTRAN Radiance	DATA
MODTRAN4OUT/TEST10.tp6	MODTRAN Tape 6 Output	DATA
MODTRAN4INP/TEST10.tp5	MODTRAN Tape 5 input	DATA

ELEVENTH TEST CASE (directory *verification/TEST_CASE_11/*)

SAMM2OUT/TEST11.BRD	SAMM2 Band radiance file	DATA
SAMM2OUT/TEST11.LOG	SAMM2 Journal file	DATA

SAMM2OUT/TEST11.OUT	SAMM2 General output file	DATA
SAMM2OUT/TEST11.SPC	SAMM2 Spectral radiance file	DATA
SAMM2OUT/TEST11.TRN	SAMM2 Transmission file	DATA
SAMM2INP/TEST11.INP	SAMM2 Input file	DATA
SAMM2ATM/DAY35N.ATM	Atmospheric file	DATA
PLOTS/modtran4_vs_samm2.png	Comparative plot	PLOT
NOTES/notes_tc11.doc	Comment	TEXT
MODTRAN4OUT/TEST11.plt	MODTRAN Radiance	DATA
MODTRAN4OUT/TEST11.tp6	MODTRAN Tape 6 Output	DATA
MODTRAN4INP/TEST11.tp5	MODTRAN Tape 5 input	DATA

The SAMM2 FORTRAN source files should be compiled and linked to make the executable version. On most UNIX machines, just typing "Makesamm2_f90" in the source subdirectory will create the "samm2_f90.exe" file which is the SAMM2 executable. "Makesamm2_f90" uses the supplied "Makefile_f90" to create and link the object files. The user should make sure that both "Makesamm2_f90" and "Makefile_f90" have execution permission.

The INTERPRETER should be compiled as a stand-alone program. INTERPRETER subroutines are described in Appendix B, and use of the program is discussed in Section 7.

The routines called binary_*.f (binary_lines.f, binary_tails.f, and binary_voigtprofile.f) convert the ASCII line parameter files to binary forms for SAMM2. The binary_*.f files should be compiled as stand-alone programs. When one of the binaries is executed, it reads the appropriate line file (SAMM96.ASC, LTETAIL.ASC or VOIGTPROFILE.ASC) and outputs a binary version of the file with the corresponding *.BIN name (SAMM96.BIN, LTETAIL.BIN, or VOIGTPROFILE.BIN). The conversion of the ASCII line files to binary files needs to be performed only once for a given platform. The ascii_*.f program can be compiled and executed to create an ASCII copy (*.ASC) of the appropriate binary file if needed for installing on another machine.

The SAMM2 installation is summarized below in Appendix AA, which contains a quick installation guide of SAMM2 on IRIX Unix platforms.

APPENDIX AA

SAMM2 QUICK INSTALLATION GUIDE
FOR IRIX f90 COMPILER

1. Copy the contents of the SAMM2 CD to your hard drive
   a. If the CD contains a single zipped and compressed file do 1b-1d; otherwise skip 1b–1d
   b. Type gunzip SAMM2.tar.gz
   c. Type tar xvf SAMM2.tar
   d. Make sure directories are created and files are placed into them
2. Change directory to SAMM2r1.8/lines/CONVERT
   a. Type make –f makebinarylines
      i. Type binary_lines.exe
   b. Type make –f makebinarylines
      i. Type binary_tails.exe
   c. Type make –f makebinarylines
      i. Type binary_voigtprofile.exe
   d. Change directory to SAMM2r1.8/lines
      i. Make sure that SAMM96.BIN, LTETAIL.BIN, and VOIGTDATA.BIN were created.
3. Change directory to SAMM2r1.8/kindir
   a. Type make –f makefileinterp
      i. Make sure interp.exe was created
   b. Make sure interp.run has execute permission
      i. Type interp.run
   c. Make sure the *.CKL files were created
4. Change directory to SAMM2r1.8/source
   a. Make sure Makesamm2_f90 has execute permission
      i. Type Makesamm2_f90
   b. Change directory to SAMM2
      i. Make sure samm2_f90.exe was created
5. Run samm2_f90.exe
   a. Your input file should be listed in SAMM2.JOBS

APPENDIX B

INTERPRETER SUBROUTINES

The INTERPRETER reads a symbolic description of an arbitrary chemical kinetics mechanism and translates it into the appropriate differential equations. The output from the INTERPRETER used by SAMM2 is an ASCII "linking" file which contains all the information describing the kinetic mechanism for a given molecular radiator.

A list of the subroutines comprising the INTERPRETER with a brief description follows.

MAIN opens the input and output files used by the INTERPRETER, and defines the following parameters used to set the maximum size of storage arrays:

KMX(=100) The maximum number of species allowed during the execution of the INTERPRETER.

LENSYM(=15) The maximum length of a species symbol.

MAXSP(=8) The maximum number of species allowed in any given reaction.

MAXTB(=6) The maximum number of third bodies allowed in any given reaction.

NRCOF(=4) The number of parameters describing the reaction rate constant.

MXLEN(=80) The maximum length of an input string.

MXLENR(=60) The maximum length of a reaction input string.

CKINTP is the driver routine which reads the species and reaction mechanism input, checks for proper syntax, and writes the "linking" file.

CKTBD checks to make sure that different third-body efficiency factors have not been input for any species.

CKINTC converts a character input string into internal code.

CKNUM converts a character string into a specified number of real numbers. The character string may contain integer, floating point, or exponential numbers separated by at least one blank.

CKSCAN scans a character string (in internal code) and converts all digits into integer numbers and all species into species indices.

CKPARS checks the input string for format errors (that is, it enforces the rules given in Subsection 3.1)

CKERR writes the error messages into the output file.

APPENDIX C

SAMM2 SUBROUTINES

A list of the key dimensional variables and subroutines comprising the various SAMM2 FORTRAN files listed in Appendix A is given below.

samm2.f   Main program and control of computations

The SAMM2 MAIN routine passes the name of the input file, normally SAMM2.INP but can be user-defined, to the top level subroutine, SAMM2. The SAMM2 routine obtains the input either in interactive or batch mode, calls the ambient and auroral chemistry modules, and then the LOS specification and radiation transport modules. It handles the selection of input/output files. The PARMS.H header file is included in SAMM2 and defines the following parameters to specify the size of various arrays and character strings.

VARIABLE	VALUE	DEFINITION
NANGMX	10	Maximum number of off-horizontal angles for covariance function.
NBINMX	50001	Maximum number of radiance bins (SPCRAD).
NBMAX	60	Maximum number of bands.
NBYMAX	102	Maximum number of atmospheric layer boundaries.
NBY2MX	500	Maximum number of LOS segments.
NCHMAX	80	Maximum length of reaction input string.
NDMAX	1000	Maximum number of lines in the defaults file.
NDELMX	20	Maximum number of grid points for the radiance covariance function.
NEDGE	4	Number of region edges.
NEDGMX	4	Maximum number of region edges.
NENVMX	2	Maximum number of environments for each region (ambient and auroral)
NFILES	3	Number of types of kinetics files (linking, states, bands).
NFIX	37	First NFIX data lines in the input file, defining information expected in the same sequence in every input file.
NIMAX	750	Maximum number of reactions.
NISOMX	8	Maximum number of isotopes for each species.
NKMAX	95	Maximum number of species allowed.
NLNMAX	15	Maximum length of a species symbol.
NMMAX	30	Maximum number of atmospheric species
NMOL	37	Maximum number of molecules.
NMOLMX	13	Maximum number of distinct radiating molecules.
NPOPMX	7	Maximum number of atmospheric profiles for a given region.
NRDMX	18	Maximum number of molecular emitters.
NREGMX	2	Maximum number of regions.
NSECMX	4	Maximum number of LOS intersections per region.
NSEGMX	18	Maximum number of major segments along the LOS.
NSINMX	5	Maximum number of solar scattering angles in the terminator region.
NSMAX	20	Maximum number of bins for band distributions.
NSPMAX	8	Maximum number of species allowed in any given reaction.

VARIABLE	VALUE	DEFINITION
NSTRMX	80	Maximum number of characters in a character string in the defaults file.
NSUNMX	50000	Maximum number of frequencies at which the solar irradiance is defined in the solar file.
NTBMAX	6	Maximum number of third bodies allowed in any given reaction.
NTMPMX	5	Maximum number of temperatures for band distributions.
NTEMPX	12	Number of temperatures for extended line tail parameters.
NVARMX	20	Maximum number of variables for generic interactive read.
NVMAX	35	Maximum number of vibrational states for each molecular emitter.
NW	200	Number of frequency bins for the Voigt line shape function.
NWMAX	200	Maximum number of frequency bins for the Voigt line shape function.
NWUSED	13	Maximum number of items presently expected to be read from a single line of the input file.
NWRTMX	20	Maximum number of types of output.
KBINMIN	490	Minimum calculational bin number for QBL algorithm.
KBINMAX	20002	Maximum calculational bin number for QBL algorithm.
SMLMX	10	Maximum length of the prefix or suffix for the lines, states, and bands files.
NAMLMX	24	Maximum number of characters for input/output file names.
DIRLMX	64	Maximum number of characters for directory path names.
LNGLMX	64	Maximum number of characters for the population file names.
MLOS	65	Maximum number of LOS's for scene generation.
MSPT	10000	Maximum number of 0.5 cm^{-1} spectral bins for QBL algorithm.
MXFLO2	2	Maximum number of standard deviations for temperature fluctuations.
MXSTAT	100	Maximum number of altitudes for which temperature statistics parameters are specified.

Several additional parameters are related to the above parameters and are automatically adjusted when the above parameters are changed. For example, the maximum number of altitude layers and the maximum number of LOS segments are related to the maximum number of layer boundaries and the maximum number of regions.

The following is a list of the FORTRAN routines with a brief explanation of each routine.

AB   returns the imaginary part of the dielectric constant.

ABSCS   determines absorption cross section for a Voigt line shape

ANDEX   computes the path refractive constant, equal to the refractive index at the specified altitude times the distance to the earth center.

ATMCNT   loads the atmospheric profiles of H_2O, N_2, O_2, and O_3 for calculation continuum absorption.

ATMCON   initializes atmospheric constants and data commons.

ACTIVE	reads the first data line in the default file to determine if the calculation is interactive or batch.
ADDRAD	is the input routine which is used to add radiative species to the ambient and auroral population calculations.
ADDREG	is the routine for reviewing, editing and adding regional information.
AEREXT	interpolates aerosol extinction, absorption, and asymmetry coefficients for the input wavenumber.
AERMRG	merges new, re-layered aerosol profile is with other layers of the atmosphere.
AERNSM	defines altitude, pressure, temperature, molecular, aerosol, cloud, and rain profiles.
AERPRF	computes density profiles for aerosols.
AITK	is the IBM scientific subroutine Aitken interpolation routine.
ALAM	computes Grun's universal energy-dissipation function using a linear interpolation of tabulated values.
ALBTRN	is part of the DISORT package which deals with the special case to get only albedo and transmissivity of entire medium as a function of incident beam angle (many simplifications because boundary condition is just isotropic illumination, there are no thermal sources, and particular solutions do not need to be computed).
ALLOLD	determines whether or not all population files are old.
ALTRIN	is part of the DISORT package which computes azimuthally-averaged intensity at top and bottom of medium.
AMBDRV	calls the appropriate subroutines to compute the enhanced vibrationally excited state populations.
AMBOUT	prints number densities for ambient molecules.
AMPERT	is for computing atmospheric fluctuations; it calls CHEMKIN routines to compute excited state populations.
APRFNU	re-layers aerosols for all four aerosol regions based on an arbitrary base, top and a scale factor for each region.
ARATE	solves the two-state steady-state equation for the atmospheric excitation rate constant.
ARCCOS	checks argument of arccosine to make sure it is between 1.0 and -1.0, then computes ACOS.
ARCSIN	checks argument of arcsine to make sure it is between 1.0 and -1.0, then computes ASIN.

ARCTAN	returns an angle between 0 and 2π given the end coordinates of a line that begins at the origin.
ARTCON	uses the kinetic data from the auroral linking file to compute the rate constants as a function of temperature in exactly the same manner as RATCON (see below). However, ARTCON identifies primary electron processes and uses the input ionization efficiencies and the ion pair production rate to compute rate constants for secondary electron formation.
ARUEXA	reads in user defined aerosol extinction, absorption coefficients and asymmetry parameters for the USS (User-Specified Spectral data) option.
ASYMTX	is part of the DISORT package which solves eigenfunction problem for real asymmetric matrix for which it is known a priori that the eigenvalues are real.
ATMDEN	loads atmospheric profile into the appropriate local arrays.
ATMFLC	generates atmospheric profiles with perturbations in kinetic temperature and total density in a single layer, leaving the remaining layers at mean values
ATMGEN	is the main driving routine to process atmospheric inputs and generate population files for ambient and auroral excited state number densities and for number density fluctuation responses to atmospheric perturbations
ATMIN	identifies the atmospheric species in the general species list, and reads atmospheric profile (containing the species number densities and kinetic temperature).
ATMLYR	computes the atmospheric properties for each layer.
ATMOUT	prints the atmospheric profile.
ATMSYM	sets up the character arrays identifying the atmospheric species and an indexing array which relates the atmospheric species to the species read by CKLINK.
AURDRV	is the driver routine for the time-dependent auroral calculation. The auroral species number densities are returned to SAMM2 main at the observation time specified by the user.
AUROUT	prints the time dependent number densities for an auroral calculation.
AZI	computes the local azimuth given the latitude of two points and the angle between them.
BANDIN	reads the molecular bands file (Subsection 3.3), which describes the line strength distribution function parameters for each vibrational transition.
BANNER	outputs the SAMM2 banner identifying the run.
BBFN	computes the Blackbody as a function of temperature and frequency.

BETABS	computes the back scatter fraction for a given asymmetry factor and cosine of angle.
BFH2O	initializes common blocks for H_2O-foreign continuum coefficients at 296 K.
BLKDTS	is BLOCKDATA located in the INPUT Module and sets numerous parameters concerning molecular data.
BLNPRO	blends available profiles to obtain the profile for the current solar zenith angle.
BLNPRO	blends profiles to interpolate across a region intersection.
BMFLUX	is the flux adding multiple scattering routine; yields upward and downward fluxes at each atmospheric layer boundary.
BNDCMP	compares the transition of a line listed on the HITRAN tape to those specified by the user.
BNDOUT	prints the line strength distribution function parameters.
BNDTRN	translates the bands selected by the user to HITRAN nomenclature.
BO2C	initializes common blocks for O_2 continuum coefficients.
BOTCHK	checks that the lowest altitude in an atmospheric profile matches that defined in block data. This assures consistency within the layer to layer pumping routine.
BRDOUT	summarizes the calculated band radiances for each transition. The number of lines used in the radiance calculation is also printed.
BS	computes interpolation parameter S such that $A=S*B(I+1)+(1.-S)*B(I)$ using a binary search routine for index I such that A is in between the array elements $B(I)$ and $B(I+1)$.
C4D	initializes common blocks for N_2 continuum coefficients.
C4DTA	returns N2 continuum absorption coefficient.
C6DTA	returns molecular Rayleigh scattering coefficient [km^{-1} @ 273 K and 1 atm] using 1999 approximation from Eric P. Shettle (NRL).
CATSTR	is a utility for the concatenation of two strings.
CFODE	is the alphabetically first of a number of CHEMKIN-derived routines which integrate the differential equations expressing the auroral model. See LSODE.
CGSUMS	increments Curtis-Godson sums.
CHECK	is a pressure and temperature conversion and error check routines.
CHECKG	checks the geometry inputs prior to a calculation.

CHEKIN	is part of the DISORT package which checks the appropriateness of input dimensions and variables for DISORT.
CHKA0	checks source and sensor LOS geometry specifications for consistency.
CHKA02	checks source and sensor LOS geometry specifications for consistency.
CHKLYR	checks that sets of boundary altitudes of multiple profiles within a region are the same.
CHKPOP	compares population file content information for consistency with region data and other profiles specified in SAMM2.INP.
CHKREG	checks all regional information, such as filenames and input variable prior to an calculation.
CHKTOP	ensures that the LOS is below the top of the atmosphere (300 km).
CIRR18	sets thickness (km), base altitude (km) and extinction (1/km) at 550 nm for standard (64 micron mode radius for ice particles) and sub-visual (4 micron mode radius) cirrus clouds.
CIRRUS	generates altitude profiles of cirrus cloud density.
CKD	computes water continuum coefficients; from LBLRTM module "CONTNM" revision 5.12 (3/24/00) uses ckd_2.4, i.e. version 2.4 of the Clough-Kneizys data.
CKLINK	reads the "linking" file created by INTERP, and defines the arrays containing information on species names, chemical kinetics mechanism (that is, the stoichiometric coefficients and the rate constants).
CKLOAD	loads the populations computed during the ambient calculation as the initial number densities for the auroral species.
CLDDTA	provides the cloud extinction and absorption data.
CLDPRF	computes density profiles for clouds / water aerosols.
CMPINT	is part of the DISORT package which calculates the Fourier intensity components at the quadrature angles for azimuthal expansion terms.
COLDEN	computes the total column density for each atmospheric layer for the radiating species.
COLMRF	calculate LOS segment data using interpolation factors for profiles, regions, and altitudes of boundaries.
COLMRF_SOL	calculate solar path segment data using interpolation factors for profiles, regions, and altitudes of boundaries.
COMOUT	prints standard comments into the defaults file.
CONABS	converts a LOS specified in latitudes and longitudes to representation in terms of solar zeniths and azimuths.

CONDTR	converts all angles to radians and transforms coordinates to the geographic coordinate system which is centered at the north pole.
CONGTM	converts coordinates based on the geographic north pole to magnetic north pole coordinates.
CONMTG	is the inverse of CONGTM.
CONREL	converts a LOS specified in terms of solar zeniths and azimuths to latitude and longitude specifications.
CONRTD	converts all angles to degrees and transforms coordinates to magnetic north pole coordinates.
CONVRT	computes concentration as a function of pressure and temperature based on 'JCHAR' unit flag.
CORLOS	estimates the atmospheric temperature correlation length along the LOS given the temperature statistic model and its atmospheric vertical and horizontal correlation lengths.
COVGEN	is the major routine for generating the numerical radiance covariance functions in both the sensor vertical and horizontal orientations.
COVHOR	estimates the local LOS contribution to the horizontal radiance covariance for a given lag in the horizontal atmospheric direction.
COVHVL	estimates the local LOS contributions to the sensor vertical radiance covariance from lags in both the vertical and horizontal atmospheric directions.
CPF12	calculates the real part of the complex probability function for a Voigt line shape.
CPYSTR	is a utility for copying character strings.
CPUSEC	is a system-dependent routine returning execution time.
CRDRIV	is the driver routine for cloud/rain models (not including cirrus and user-defined cloud extinction and absorption).
CRMERG	merges together cloud/rain and old atmospheric profiles. Layer boundaries are merged together if they differ by less than half a meter.
CROSS	takes the cross product between two vectors using the right hand rule.
CRPROF	defines cloud/rain model profiles.
CRSPEC	defines cloud particle spectral data.
CRUPRF	reads in user-defined cloud/rain profiles.
CRUSPC	defines user-defined cloud spectral data.
D1MACH	See LSODE.

DAXPY	See LSODE.
DAY	calls a system-dependent routine to determine the date and time of the SAMM2 run. The actual call is commented out of the subroutine.
DAZI	is a double precision version of AZI.
DCHECK	checks for the existence of a directory.
DDOT	See LSODE.
DEBYE	Calculates wavenumber dependence of dielectric constant of water.
DEFALT	Interpolates profiles from the 6 built-in model atmospherics in MODTRAN to altitude Z.
DEFMOM	defines area-averaged ground BRDF azimuth Fourier moments.
DESATT	calculates the attenuation coefficients and asymmetry parameter for the desert aerosol based on the wind speed and meteorological range.
DEVCBD	defines the file unit numbers for MODTRAN output as the SAMM2 journal file.
DEWV	computes the equivalent width for a single isolated Voigt line.
DFLTSG	reads the regional information found in the defaults file.
DGBFA	See LSODE.
DGBSL	See LSODE.
DGEFA	See LSODE.
DGESL	See LSODE.
DISBBF	is part of the DISORT package which computes the Planck black body function [$W/cm^2/sr/cm^{-1}$] as a function of T and wavenumber.
DISORT	Plane-parallel Discrete Ordinates Radiative Transfer (DISORT) PROGRAM. This program, developed by Stamnes *et al.* [W. Wiscombe, K. Stamnes, S.-C. Tsay and K. Jayaweere, *Applied Optics*, **27**, 2502-2509, 1988], is essentially used as a black box (i.e., without change). MODTRAN used DISORT to get MS source function for each atmospheric layer.
DLATI	is a double precision version of LATI.
DLONGI	is a double precision version of LONGI.
DOP	returns the real part of the dielectric constant.
DOT	takes the dot product of two vectors.
DSCAL	See LSODE.
DSTDTA	initializes commons containing the desert aerosol extinction and absorption coefficients, and asymmetry parameters.

DUMPDE	writes the current values of the input variables into the defaults file.
DWIDTH	calculates the Doppler halfwidth.
E2	computes the second exponential integral as a function of optical depth.
EMISS	locates the Einstein A coefficient for the current transition, and also calculates the sum of all Einstein A coefficients for all transitions from the upper vibrational state.
EPFLUX	calculates the primary energy flux assuming either a Gaussian or Maxwellian distribution function for the electron spectra.
ERATE	calculates the earthshine excitation rate for each atmospheric layer.
ERRMSG	prints an error messages.
ESHINE	calculates the earthshine flux for the current transition using the specified effective earthshine temperature.
EWSET	See LSODE.
EXABIN	loads extinction, absorption and asymmetry coefficients for the four aerosol altitude regions.
EXPINT	performs an exponential interpolation; linear, if either function value is non-positive.
EXPLEN	estimates the exponential scale length of a numerical covariance function, by estimating the lag where the covariance is decreased by a factor of $1/e$.
EXTDTA	initializes commons containing aerosol extinction coefficients for different altitude regions.
FBETA	calculates the path zenith angle for the observer and source using refractive geometry.
FCHECK	opens files and checks their status against the expected status. For example, does a new file already exists.
FILPRO	selects the extended region profile for multiple scattering calculations.
FIND	estimates by linear interpolation an intermediate value of a function when supplied a grid of numerical values.
FIND1	is identical to find except for calling arguments. It also returns the grid point which is closest to the interpolated value.
FINDEX	tries to find an exact index match for a variable within a specified tolerance (similar to subroutine HUNT).
FITALL	performs non-linear least squares fitting.
FLAYZ	determines the layer boundaries when one of the model atmospheres is selected.

FLCFIL	opens output files for intermediate and final results of the perturbations of ground and excited state number densities.
FLCGEN	determines the responses of molecular state number density to fluctuations on atmospheric temperature fluctuations.
FLG4PT	performs a 4-point Lagrange interpolation for z between z_2 and z_3, inclusive. The abscissas must be monotonic, $z_1 < z_2 < z_3 < z_4$ or $z_1 > z_2 > z_3 > z_4$.
FLUXES	is part of the DISORT package which calculates the radiative fluxes, mean intensity, and flux derivative with respect to optical depth from the M=0 intensity components (the azimuthally-averaged intensity).
FNDCOL	provides the data necessary for computing the column amounts for each segment along the LOS.
FNDCOL_SOL	provides the data necessary for computing the column amounts for each segment along the solar path.
FNDH2	calculates the source location, altitude, and zenith angle, and minimum altitude and location along the LOS.
FNDPRO	determines the atmospheric region in which a point along the LOS is located and the relevant atmospheric profile, and result atmospheric properties at the point.
FRN296	loads foreign continuum at 296 K.
FORMV	calculates the Voigt line shape function.
FRQ5DT	defines the layer independent 5 cm^{-1} spectral data for MODTRAN continuum parameters.
FTRANG	calculates the path zenith angle for the observer and source using refractive geometry.
FUN	supplies LSODE with the species production rates obtained from PRAT.
FUNCO	computes the current value of a non-linear least squares estimate given the current non-linear parameters.
FUNF	is an external function called by the pattern search routine to compute the current value of the function being minimized.
GAMFOG	computes attenuation of equivalent liquid water content in clouds or fog.
GAMMA	computes the gamma function.
GAMMAR	computes ratios of gamma functions of arguments that differ by one half.
GEOTOP	determines LOS geometry specifications for the sensor above at or below the highest altitude in the atmospheric profile.
GEMOUT	writes out a brief summary of the LOS information to SAMM2.OUT.
GENOUT	writes out a brief general description of each regional calculation.

GENTAB	generates the proper character string for appending to a standard population file name.
GEOMEX	calculates the full, over-specified set of variables which describe the LOS.
GEOMRF	uses the allowable set of geometry input parameters to compute region intersections, multiple atmospheric profiles, and structure LOS segmentation using refractive geometry.
GETAZI	handles interactive input of local azimuth angles for a LOS.
GETLOC	interactively determines a LOS in either latitude and longitude representation or solar zenith and azimuth terms.
GETLOS	is the inverse of PUTLOS; it gets LOS parameters from arrays.
GETSOL	handles interactive input of the point beneath the sun in latitude and longitude.
GMRAIN	computes attenuation of condensed water in form of rain.
GNDGEN	defines the ground reflectance properties.
GRFGEO	update the geometric LOS properties with refractive geometry effects.
GRIDINT	maps (linear or exponential) a tabulated function stored in Y_1 for corresponding values of the independent variable stored in X_1 and interpolates them onto a new grid of values for the independent variable stored in X_2. The result is stored in array Y_2.
GTBRDF	reads in BRDF parameters and calculates required reflectance integrals using the BRDF function, BRDFUN. If successful, GTBRDF returns a value of TRUE.
GTSURF	returns surface reflectance/emittance values at specified wavelength.
GTWAL	reads in Walthall BRDF parameters and calls function WALTHL to perform analytic integrations of the WALTHALL BRDF. If successful, returns a value of TRUE.
GVLOAD	transfers number densities, vibrational transitions, and related information from regional arrays into global ones, which are ultimately used by SPCRAD.
GVZERO	initializes all of the global variable arrays.
HEADER	writes header of information into the scene generation interface files, the 2D and 3D files.
HENGNS	calculates the Henyey-Greenstein scattering phase function.
HERTDA	computes the Herzberg O_2 absorption coefficient.
HORGEN	computes the contributions to the horizontal radiance covariance distribution function.
HUNT	finds the two bounding indices of a variable in a monotonic array.

IDAMAX	See LSODE.
IMSTAT	is the interactive input routine for description of temperature statistics model.
INAER	is the interactive input routine for reviewing/changing aerosol physical and optical properties.
INATM	is the interactive input routine for reviewing/changing the user's choice of model atmosphere.
INAUR	is the interactive input routine for reviewing/changing the user's choice of auroral conditions.
INBOND	is the interactive input routine for inputting the parameters which define a local region.
INCGEO	increments the refractive path geometric data.
INCLD	is the interactive input routine for reviewing/changing cloud physical and optical properties.
INDX	returns the refractive (real and imaginary parts) index of water.
INGEOM	reads LOS geometry information from the default file and allows the user to review/change the parameters.
INMOL	is the interactive input routine for reviewing/changing the radiators included in the population calculations.
INMULT	is the interactive input routine for reviewing/changing the multiple scattering options.
INNAME	is the interactive input routine for reviewing/changing the names for the standard input and output files.
INNEM	is the interactive input routine for reviewing/changing the input parameters for the Monte Carlo radiation trapping module.
INOUT	allows the user to review and/or modify the amount of output written to the general output file.
INPOP	is the interactive input routine for reviewing/changing the population file names and status.
INREGN	is the main interactive input routine for reviewing/changing regional information.
INSIDE	determines whether the local region forms a proper convex spherical pyramid.
INSOL	is used to change/review the solar zenith angle.
INSOURC	is the interactive input routine for reviewing/changing the solar irradiance file, and selecting the extra-terrestrial source (sun or moon).

INSPEC	is the interactive input routine used to change and/or modify the spectral range, resolution and species included in spectral radiance calculation.
INSTAT	is the interactive menu routine for input of temperature statistics options.
INSTDS	supplies the menus for input of name patterns and directories for kinetics, atmospheric, population and lines files.
INSURF	is the interactive input routine for reviewing/changing the ground reflectance properties.
INTCLN	estimates the integral correlation length (angle) from a sample of a numerical covariance function.
INTCOR	is part of the DISORT package which corrects intensity field by using Nakajima-Tanaka algorithm.
INTDY	See LSODE.
INTITL	is the interactive input routine for reviewing/changing the title of the calculation.
INTYPE	is the interactive input routine used to change the environment type. SAMM2 currently has two environments: ambient and auroral.
IPATH2	is the interactive menu routine for input of sensor to source LOS specifications.
IPATH3	is the interactive menu routine for input of sensor to space LOS specifications.
IPATH4	is the interactive menu routine for input of limb LOS specifications.
IPATH5	is the interactive menu routine for input of multiple sensor to source LOS specifications.
IPATH6	is the interactive menu routine for input of multiple sensor to space LOS specifications.
IPATH7	is the interactive menu routine for input of multiple limb LOS specifications.
IPPRAT	calculates the ion pair production rate as a function of altitude for the specified auroral energy parameters.
ISAMAX	is part of the DISORT package which finds the maximum absolute value of the element of a vector by examining the elements spaced by a specified increment.
ITOASC	converts an integer to its ASCII representation.
JAC	supplies LSODE with the Jacobian of the species production rates obtained from PRATJ.
JOU	converts JCHAR flags ('1' through '6', ' ', and 'A' through 'K') into integers (1 through 6,10 and 10 thorough 20).

KEEPI	stores a copy of an integer vector.
KEEPR	stores a copy of a real vector.
LATI	computes the latitude of point "I" in radians given the latitude of another point, "II" and the latitude of point I to II.
LATPHI	calculates the latitude and longitude of vector 2 relative to vector 1, given the latitudes and longitudes of vectors 1 and 2 relative to a common vector.
LAYCLD	determines cloud density and rain rate for a layer.
LAYERS	calculates the refractive path between two altitudes.
LAYVSA	returns haze information for VSA (Vertical Aerosol Algorithm) option.
LCTRIM	removes leading and trailing blanks from a character string.
LENSTR	determines the non-blank length of a character string.
LEPOLY	is part of the DISORT package which computes the normalized associated Legendre polynomial, defined in terms of the associated Legendre polynomial.
LINRD	reads the binary line parameter file, one line at a time.
LNTRP	performs a linear interpolation between (x_a, y_a) and (x_b, y_b); find value at x.
LOADAER	uses the necessary MODTRAN routines to set up the aerosol and cloud profiles and their optical properties. It is based on routine DRIVER from MODTRAN.
LOADDE	opens and loads the input data found in SAMM2.INP into the array DFLTS. If SAMM2.INP is not found, NODFTS is called to load a set of default parameters.
LOADTS	loads temperature statistical information for quick relayering of the atmosphere. Routine is called by ATMGEN.
LOCALTAIL	computes contributions from line tails (and their temperature derivatives) to LOS segment optical depths (and their temperature derivatives) for spectral bin containing the emission line and its nearest spectral bin.
LOCALTAILV	computes line tails contributions to vertical path or solar path segment optical depths for spectral bin containing the emission line and its nearest spectral bin.
LOCASE	converts a character string to lower case.
LOCATE	calculates the latitude and longitude of a point along the LOS.
LONGI	computes the longitude of point "I" in radians given the longitude of another point, "II" and the longitude of point I to II.
LOOPDT	outputs numerical estimate of a modified Bessel function approximations to the radiance covariance function.

LOS	determines the LOS vector.
LOWIN	reads the continuum files for lower-atmosphere solar radiation propagation.
LOWOUT	writes the continuum information to the output file.
LSODE	The LSODE package numerically integrates the auroral rate equations. It uses Gear's method for stiff differential equations and is supplied with the Sandia CHEMKIN code. The following routines are used by the LSODE package: INTDY, STODE, CFODE, PREPJ, SOLSY, EWSET, VNORM, DGEFA, DGESL, DGBFA, DGBSL, DAXPY, DSCAL, DDOT, IDAMAX, DIMACH, XERRWV.
LSODED	See LSODE.
LUBKSB	performs the backsubstitution for the LU decomposition procedure to solve a set of simultaneous linearly independent algebraic equations (the steady-state equations).
LUDCMP	performs the matrix decomposition for the LU decomposition procedure to solve a set of simultaneous linearly independent algebraic equations (the steady-state equations).
LWIDTH	calculates the Lorentz halfwidth.
LWRITE	computes logical variable used as switches for writing various output.
LYRPRP	integrates through the atmospheric layers to determine the escape probabilities and single-scattering enhancements.
LYRENH	calculates the nth-order multiple scattering enhancement to the excited-state number density using the single-scattering enhancement matrix.
MAIN	is the multiple jobs calling program for SAMM2. Opens the SAMM2.JOBS file, reads the list of SAMM2 input files then sequentially calls SAMM2 to process each input file.
MAJSEG	determines the major segments of the LOS through a region.
MARDTA	provides the marine aerosol absorption and extinction data.
MARINE	determines Aerosol extinction + absorption coefficients for the Navy maritime model.
MCHECK	checks the range of the variable to verify that the variable value is between the given bounds.
MDTA	provides the cloud density and rain rate data.
MKFNAM	is an utility for creating a file name with suffix and a full directory path.
MLATMB	provides the atmospheric profile data for the 6 built-in MODTRAN atmospheres.

MLTSCT	is the driver for the multiple scattering calculations in SAMM2. This routines sets up and calls the appropriate routine to calculate the multiple scattering contribution to the radiance source term. Depending on the value of the flag: DIS, either the two-stream model or the DISORT multiple stream model is used.
MODLOS	gets the LOS properties necessary to call refractive path routines.
MOLSCT	returns molecular scattering phase function spectral parameters.
MRGSTR	merges a character string with another string.
MSCOUT	writes out multiple scattering information, i.e., physical characteristics of aerosols and clouds.
MSGEOM	calculates solar and scattering angles for the multiple scattering routines and/or ground reflection model.
MSRAD	sets up optical properties profiles for vertical path then calls DISORT which returns ms source functions.
MSSOLR	is part of the DISORT package which outputs multiple scattering solar source function, and downward diffuse solar flux at surface.
MSTHML	is part of the DISORT package which outputs multiple scattering thermal source function, and downward diffuse thermal flux at surface.
N2FAC	computes the effective rate constant for the $CO_2(00011)+N_2(0)$ quenching process and the excited state populations for N_2 following Kumer and James.
NEMDRV	is the driver routine to compute the escape probabilities and enhanced excited-state number densities for each atmospheric layer using Monte Carlo integration of atmospheric layers, line strengths, and frequencies.
NEMFAC	computes the probability of escaping a specified layer and the excitation of the layer from all other layers. These quantities are used for the subsequent auroral calculation.
NEMOUT	prints out some of the inputs used by NEMESIS.
NEMRXN	identifies the excitation and relaxation processes in the chemical kinetics mechanism for the current transition being considered by NEMESIS.
NODFTS	loads the default values for a calculation into SAMM2.INP when an SAMM2.INP is not found.
NORM	normalizes a 3 vector.
NOVAER	reads the output of the self-standing NOVAM aerosol model program.
NOVMRG	merges together NOVAM layers with cloud/rain and old atmospheric profiles. Layer boundaries are merged together if they differ by less than half a meter.
NUNIT	determines an unused file unit number between 10 and 99.

O2CONT	provides the O_2 continuum data for frequency 1395-1760 cm^{-1}.
O2INF2	provides the O_2 continuum based on the formulation of Mlawer et al. over the spectral region 9100-11000 cm^{-1} [Mlawer, Clough, Brown, Stephen, Landry, Goldman, & Murcray, "Observed atmospheric collision-induced absorption in near infrared oxygen bands," *J. Geophys. Res.*, **103**, 3859-3863, 1998].
O2INT	Interpolates over frequency of the continuum data.
O2MATE	provides the O_2 continuum based on the formulation of Mate *et al.* over the spectral region 7550-8486 cm^{-1} (adapted from LBLRTM [B. Mate, C. Lugez, G.T. Fraser, and W.J. Lafferty, "Absolute intensities for the O_2 1.27 micron continuum absorption", *J. Geophys. Res.*, **104**, 30,585-30,590, 1999]).
O3CHAP	provides the absorption coefficient for the O_3 Chappuis and Wulf band, 9170-2456 cm^{-1}.
OPENS	is an utility which opens the file containing the modified bessel function approximation to the radiance covariance function.
OPSANG	computes the supplemental angle.
OPTDEP_QBL	computes total contributions to LOS segment optical depth, NLTE source term and their temperature derivatives at 0.001 cm^{-1} resolution for spectral bin containing the emission line and its nearest spectral bin .
OPTDEP_SOL	computes total contributions to solar path segment optical depth and NLTE source term at 0.001 cm^{-1} resolution for spectral bin containing the emission line and its nearest spectral bin.
ORDKEY	determines the relative order of the elements of a vector, and returns an integer vector key containing the element indices in order of increasing element magnitude.
OZENMX	checks the consistency of input source altitude and observer zenith.
POPN2O2	calculates the LTE excited state populations for N_2 and O_2.
PARSEC	separates text and numerical input parameters from an input character string.
PAT	is the major subroutine for performing pattern search non-linear optimizations.
PICKSJ	determines the line strength selected from the line strength distribution function.
PICKZ	finds the initial location and the corresponding layer for photon emission.
PLKAVG	is part of the DISORT package which computes Planck function integrated between two wave numbers.
POLL	contains the main interactive menu for running SAMM2.
POPIN	reads in population file data for CHKPOP.

POPLTE	computes the LTE vibrationally excited populations.
POPOUT	outputs the number densities as a function of altitude for each vibrational state in the mechanism.
PRAT	uses the data obtained from the "linking" file to set up the differential equations for the species production rates.
PRATJ	uses the data obtained from the "linking" file to set up the Jacobian of the species production differential equations with respect to the species number densities.
PRAVIN	is part of the DISORT package which prints azimuthally averaged intensities at user angles.
PRFDTA	provides the aerosol profile number densities.
PREPJ	See LSODE.
PRFINT	interpolates a MODTRAN default cloud/aerosol profile onto SAMM2 altitude grid.
PROBDF	is the main driver for the interactive menu or batch execution of SAMM2. This routine determines all of the input parameters for a SAMM2 calculation.
PRTINP	is part of the DISORT package which prints values of input variables.
PRTINT	is part of the DISORT package which prints the intensity at user polar and azimuthal angles.
PRTROT	calculates the rotational partition function.
PUTLOS	is the inverse of GETLOS; it puts modified LOS parameters back into arrays.
QBLINIT	initializes parameters for line cloning approach used in QBL calculation.
QGAUSN	is part of the DISORT package which computes weights and abscissas for ordinary Gaussian quadrature (no weight function inside integral) on the interval (0,1).
QUADRI	finds quadratic fit to a numerical function.
QUENCH	computes the total quenching rate for the upper state of the transition.
RADE	computes the earth radius as a function of latitude.
RADIN	reads the molecular states file (Subsection 3.2), which contains the molecular radiator, the vibrational states included in the mechanism and the transitions to be considered by NEMESIS and SPCRAD.
RADOUT	outputs the information contained in the molecular states file.
RADREF	computes the inverse of the radius curvature of a refracted ray for a horizontal path.

RAIN	computes optical properties of rain.
RANDOM	generates uniformly distributed random numbers between 0 and 1.
RANGER	computes the over-complete set of LOS geometry parameters.
RATCON	uses the kinetic data from the linking file to compute the rate constants as a function of temperature. The assumed form of the rate constant is $k = A\,T^B \exp(-E/T - C/T^{1/3})$, where A is the pre-exponential factor, B is the exponent of the temperature term, E is the activation energy (can also be used to write a reverse rate constant in terms of the forward rate constant via detailed balance), and C is the (historic) SSH $T^{1/3}$ coefficient.
RATIO	is part of the DISORT package which calculates ratio of two reals with over- and under-flow protection.
RATMOD	modifies the Einstein A-coefficients and loads the layer excitation rates into the appropriate rate constant arrays. These quantities are computed by the ambient calculation.
RCHECK	checks the range of the variable to verify that the variable value is between the given bounds.
RDBRDF	reads in the surface BRDF (Bidirectional Reflectance Distribution Function) type. If a problem occurs, a value of .FALSE. is returned.
RDEXA	reads in user defined extinction absorption coefficients and asymmetry parameters.
RDLAMB	reads in the Lambertian surface integer label or surface name and calls RDSALB to read in the spectral data. If a problem occurs, a value of .FALSE. is returned.
RDNSM	reads MODEL 7 DATA (user-specified MODTRAN atmosphere) when the VSA (Vertical Structure Algorithm) aerosol is chosen.
RDSALB	reads in the Lambertian surface spectral albedo data.
REDCHR	reads user response to queries that require character string answers.
REDINT	reads user response to queries that require integer answers.
REDREL	reads user response to queries that require real variable answers.
REFHAP	returns the 3-parameter Hapke 1981 model Bidirectional Reflectance Distribution Function (BRDF).
REFPV	returns the 4-parameter Pinty and Verstraete 1991 Model Bidirectional Reflectance Distribution Function (BRDF).
REFRAH	returns the 3-parameter Rahman model Bidirectional Reflectance Distribution Function (BRDF).
REFRL	returns the 5-parameter Ross-Li (reciprocal Ross thick Li sparse) model Bidirectional Reflectance Distribution Function (BRDF).

REFROU	returns the 3-parameter Roujean model Bidirectional Reflectance Distribution Function (BRDF).
REFWAL	returns the 4-parameter Walthall model Bidirectional Reflectance Distribution Function (BRDF).
REFWLS	returns the 4-parameter sinusoidal Walthall model Bidirectional Reflectance Distribution Function (BRDF).
REGANG	maps an arbitrary angle to a specified interval of 2π.
REGCHK	checks region altitude boundaries for consistency with profile boundaries.
REGDTR	converts edge latitudes and longitudes to radians and converts to geographic coordinates if necessary.
REGLOS	determines if observer or source is inside the angular region.
RELABS	performs interconversion of relative and absolute LOS specifications.
RETOUT	writes a summary of the population file to SAMM2.OUT when an old population file is used in a new calculation.
RETREV	reads the saved population file data.
RFCCLO	is an utility for closing radiance statistics intermediate and output files.
RFCFIL	is an utility for opening radiance statistics intermediate and output files.
RFDEX	computes the profile of the refractive index-1 for the average value of the minimum and maximum input frequency.
RFLECT	is the driver for defining the surface reflectance properties.
RFPRO	obtains the H_2O profile and calls RFDEX for profile of the refractive index.
RFRACT	returns the refractivity, defined as one minus the real part of the index of refraction.
RIGHT	determines the smallest single and double precision values that can be added to one and produce a number greater than one.
RMRAD	eliminates a radiator from the list of species desired for population calculation.
RMREG	is used to remove an unwanted region.
RNSCAT	returns optical properties for rain for frequency less than 250 cm^{-1}.
RPATH	is the driver routine to obtain the refracted path from observer to target or space.
RPATH_SOL	traces refractive ray from LOS segment to sun.
RSOUT	write out radiance statistics.

RVLOAD	transfers the number densities, vibrational transitions, and related information from the local environment arrays into regional arrays.
RVZERO	initializes all regional variable arrays.
SAMM2	is the main subroutine of SAMM2.
SASUM	is part of the DISORT package which sums elements of a vector from 1 to N-1 spaced by a selected increment.
SAV1D0	is part of the DISORT package which saves vector X in another vector; both start at index 0.
SAV1D1	is part of the DISORT package which saves vector X in another vector; both start at index 1
SAVE	writes the population file.
SAXPY	is part of the DISORT package which is a vector manipulation routine: SY and SX are two input vectors, and the output is SY, which is a liner combination of SY and SX.
SCALHT	calculates the reciprocal of the scale height.
SCNFLX	degrades (and outputs) the spectral flux with a scanning function.
SDOT	is part of the DISORT package which returns the dot product of two vectors SDRIVE organizes the radiation transport output and the temperature model to facilitate the calculations of radiance statistics driver of the radiance statistics routines.
SDRIVE	is the driver routine for the calculation of the radiance covariance function.
SECSCA	is part of the DISORT package which computes the secondary scattered intensity.
SEGGEN	generates minor segments for each major segment along the specified LOS.
SEGMNT	computes major segment properties, including the major segment lengths, the number of major segments, and identifies the lower boundary for each segment.
SEPARA	determines the grid of distances (separations) based on an input angular grid and a range from the observer to the tangent point.
SETDIS	is part of the DISORT package which performs miscellaneous setting-up operations for DISORT.
SETGEO	initializes geometry parameters.
SETMTX	is part of the DISORT package which calculates coefficient matrix for the set of equations obtained from the boundary conditions and the continuity- of-intensity-at-layer-interface equations.

SETUPS	estimates the structure scale and tolerances for the estimate of the covariance function.
SF260	provides the data for the H_2O self continuum at 260 K.
SF296	provides the data for the H_2O self continuum at 296 K.
SGBCO	is part of the DISORT package which factors a real band matrix by Gaussian elimination and estimates the condition of the matrix.
SGBFA	is part of the DISORT package which factors a real band matrix by elimination.
SGBSL	is part of the DISORT package which solves for X in $A * X = B$, where A is a band matrix, B and X are vectors.
SGECO	is part of the DISORT package which factors a real matrix by Gaussian elimination and and estimates the condition of the matrix.
SGEFA	is part of the DISORT package which factors a real matrix by Gaussian elimination (called by SGECO).
SGESL	is part of the DISORT package which solves the real system: $A * X = B$ or $TRANS(A) * X = B$, using the factors computed by SGECO or SGEFA.
SHOGEO	writes the current LOS geometry inputs to the screen.
SHOLOS	writes to the screen all LOS information at the end of a LOS menu session.
SHOZEN	writes to the screen all LOS solar zenith information at end of a menu session.
SINSCA	is part of the DISORT package which computes the singly scattered intensity.
SINT	interpolates over frequency of the continuum data.
SINTRP	performs a linear interpolation to obtain the line strength distribution function for the appropriate layer temperature.
SLF260	computes the H_2O self continuum coefficient at 260 K for a given frequency.
SLF296	computes the H_2O self continuum coefficient at 296 K for a given frequency.
SLFTST	is part of the DISORT package which, If COMPAR=FALSE, saves user input values that would otherwise be destroyed and replace them with input values for self-test. If COMPAR=TRUE, compare self-test case results with correct answers and restore user input values if test is passed.
SMOOTH	is a smoothing routine used by COVGEN.
SNCMS	computes azimuthally-dependent layer solar source functions.
SOLARPATH	driver routine for RPATH_SOL.
SOLEIG	is part of the DISORT package which solves eigenvalue/vector problem necessary to construct homogeneous part of discrete ordinate solution.

SOLFLX	calculates solar flux at a transition frequency assuming a 5500 K blackbody.
SOLSY	See LSODE.
SOLVE0	is part of the DISORT package which constructs right-hand side vector -b- for general boundary conditions and solve system of equations obtained from the boundary conditions and the continuity-of-intensity-at-layer-interface equations.
SOLVE1	is part of the DISORT package which constructs right-hand side vector -B- for isotropic incidence (only) on either top or bottom boundary and solve system of equations obtained from the boundary conditions and the continuity-of-intensity-at-layer-interface equations.
SOLZEN	stores the cosine of the solar/lunar zenith angle data for the multiple scattering calculations.
SOURCE	returns solar or lunar irradiance [$W/cm^2/cm^{-1}$]. Corrections are made for the sun's elliptic orbit. If the source is the moon, the phase angle between the sun, moon and earth is taken in account.
SPALTR	is part of the DISORT package which calculates spherical albedo and transmissivity for the entire medium from the M=0 intensity components; this is a very specialized version of FLUXES.
SPCBININIT	initialize arrays of LOS segment optical depths, NLTE source terms and their temperature derivatives for current spectral bin.
SPCBININIT_SOL	initialize arrays of solar path segment optical depths and NLTE source terms for current spectral bin.
SPCCHK	checks to ensure that populations exist for all species selected for spectral calculation.
SPCFLX	outputs the spectral flux degraded with a triangular slit function.
SPCDEG	degrades the high-resolution spectral radiance and transmission with a triangular slit function.
SPCOUT	writes the spectral radiance as a function of wavenumber to SAMM2.SPC.
SPCQBL	is the main spectral radiance routine called by the main SAMM2 routine. It calls LINRD to read an individual line, calls BNDCMP to determine if this line is for a user-selected transition, and calls ROT/ROTVIB to perform the LOS radiance calculation. The end result from SPCRAD is the spectral radiance for a line which is stored in array RADBIN.
SRATE	calculates the solar excitation rate for each atmospheric layer.
SRTMOL	sorts molecular radiators according to AFGL molecule number.
SSCAL	is part of the DISORT package which scales elements, spaced by a specified increment, of a vector by a scalar.

SSRLYR	overlays the MS source function calculation for the MODTRAN atmospheric layers on that used in SAMM2.
SSOURCE	drives QBL calculations of solar path segment optical depths and NLTE source terms.
STATIN	routine is for reading altitude dependent temperature statistics from a file.
STDMDL	loads one of the 6 standard atmospheric profiles into a common block and calculates the densities of the various absorbing gases and aerosols.
STEADY	sets up the steady state rate equations and then uses LUDCMP and LUBKSB to solve the set of linear algebraic equations for the number densities ck. The major limitation to the steady-state procedure used here is the assumption that the rate equations are linear in the unknown vibrational population, that is, there is no energy exchange among the emitting species. This restriction can be easily relaxed by using an algorithm which solves nonlinear equations (as opposed to LUDCMP/LUBKSB).
STODE	See LSODE.
STUFFD	fills dflts array with regional input information.
SUBSOL	computes solar latitude and longitude from the date and time of day, during interactive input.
SUMOUT	prints a calculational summary at the beginning of each SAMM2 run.
SUNIN	reads the solar irradiance file and stores the data in SUN array.
TAB	computes the power law coefficients for the absorption coefficient for the Marshall-Palmer water drop size distribution.
TAUEFF	is called by AMPERT for determining effective optical depth.
TERPEV	is part of the DISORT package which interpolates eigenvectors to user angles.
TERPSO	is part of the DISORT package which interpolates source functions to user angles.
TIMDEP	controls the time dependent integration of the auroral rate equations.
TANHT	calculates the tangent height along a refracted path.
THMFLX	calculates the vertical flux assuming no atmospheric or surface scattering.
TITLE	loads title information for clouds and aerosols, as well as default visibilities.
TNRAIN	calculates transmission due to rain as a function of rain rate (mm/hr), or within 350 cm^{-1} uses the microwave table routine to obtain the extinction due to rain.
TRANIN	reads the states file to determine which transitions are to be considered by SPCRAD. It is only called when retrieved population files are being used.

TRLAY	calculates parameters for solar hybrid modified delta Eddington 2-stream approximation. The equations are derived from W. E. Meador and W. R. Weaver, *J. Atmos. Sci.*, **37**, 630-642, 1980. This routine is needed by BMFLUX.
TSOUT	outputs atmospheric temperature statistics to the SAMM2 output file.
TSTBAD	is part of the DISORT package which writes name of variable failing self-test and its percent error from the correct value; returns .FALSE.
UNIVEC	determines the unit vector from latitude and longitude.
UPBEAM	is part of the DISORT package which finds the incident-beam particular solution.
UPCASE	converts a character string to all upper case characters.
UPISOT	is part of the DISORT package which finds the particular solution of thermal radiation.
USRINT	is part of the DISORT package which computes intensity components at user output angles for azimuthal expansion terms.
VSANSM	provides atmospheric properties for VSA algorithm.
VBININIT	initialize arrays of vertical path segment optical depths for current spectral bin.
VBTOUT	outputs the vibrational temperatures as a function of altitude for each vibrational state in the mechanism.
VECPOL	determines a Cartesian vector from an altitude, latitude and longitude.
VECVRT	determines polar coordinates from a Cartesian vector.
VERGEN	computes the contributions to the vertical radiance covariance distribution function.
VIBES	converts vibrational assignments in the HITRAN 92 format to the 85 format when ICHOIC=1. When ICHOIC=2 it converts 85 formats to the 92 ones. This routine is from the HITRAN line selection program.
VIBTMP	calculates vibrational temperatures of excited- state species.
VNORM	See LSODE.
VODQBL	drives QBL calculations of the vertical path segment optical depths required in Multiple Scattering (MS) routines.
VODRLYR	overlays vertical path segment optical depths calculated with SHARC layer grid onto MODTRAN grid, for MS calculations.
VOPTDEP_QBL	computes total contributions to vertical path segment optical depth for spectral bin containing the emission line and its nearest spectral bin.

VOIGT	determines the emission frequency using a Voigt line shape function. The absorption cross section at this frequency is also computed.
VOIGTINIT	read the Voigt line shape parameters.
VOIGTPROFILE	compute the Voigt line-shape profile using the parameters from the arrays setup in VOIGTINIT.
VSANSM	outputs pressure, temperature and various atmospheric species at common layers.
VSA	provides the Vertical Structure Algorithm for aerosols.
WALTHL	calculates surface reflectance values using a Walthall BRDF model. If successful, a value of .TRUE. is returned.
WATVAP	computes water vapor mass density (gm/m^3) given humidity (dew point or relative humidity), partial pressure, mass density (gm/m^3) or mass mixing ratio (gm/kg).
WINTHP	performs the LOS numerical integration to obtain the horizontal radiance covariance distribution function.
WINTVP	performs the LOS numerical integration to obtain the vertical radiance covariance distribution function.
WLTHLS	calculates surface reflectance values using a modified Walthall BRDF model - the zenith angles are replaced by their sine function. If successful, a value of .TRUE. is returned.
WRTBAD	is part of the DISORT package which writes names of erroneous variables and returns .TRUE.
WRTDIM	is part of the DISORT package which writes name of too-small symbolic dimension and the value it should be increased to; return 'TRUE'; used by CHEKIN.
WRTGEO	writes LOS geometry specifications to menu screen.
WRTLOS	writes LOS demarcation lines in files to separate multiply LOS records.
WRTOUT	is an utility for writing records to the terminal screen or to the standard output file.
WRTSTR	writes a character string to an internal file.
WTLFT	returns the weight of the left side of a triangular slit function.
WTRGT	returns the weight of the right side of a triangular slit function.
WTSUM	outputs the spectral flux degraded in SCNFLX.
XERRWV	See LSODE. Prints LSODE-related error and warning messages.
XIFUNC	is part of the DISORT package which computes function of layer optical depth.

XMLATM	provides the spectral data for molecules whose absorption coefficients are represented by cross section data rather than line parameters.
XNTRP	performs exponential interpolation between (x_1, y_1) and (x_2, y_2); find value at x
XNUM	translates an alphanumeric character string containing N integer, real, or exponential numbers into their respective real values.
XTAILINIT	initializes parameters for extended line tail contributions.
ZEROAL	is part of the DISORT package which initializes a larger number of arrays to zero.
ZEROIT	is part of DISORT, initializes a real array to all zero.
ZMRG2	merges A and B to create the merged array A by eliminating redundants and preserving order.
ZMRG	merges two arrays and create a new array; also eliminate redundants (within tolerance) and preserve order.
ZNFDGE	determines the appropriate profile column densities for each segment of the LOS.
ZNUKNU	computes the product of the argument raised to the power (nu) times the modified Bessel function of the second kind of order (nu).

APPENDIX D
TEST CASE VERIFICATIONS

SAMM2 is supplied with eleven test cases that have been verified against the earlier SHARC4.1, SAMM1.1, or MODTRAN4 codes. These eleven test cases allow the user to check that SAMM2 has been properly installed, and to demonstrate some of its features. The input files which define these cases are supplied. Apart from minor round off error, if the user employs the data files supplied, the resulting calculation outputs should match those shipped for the cases. Appendix A lists the files shipped for each case. The main points of interest for each case are discussed here.

SAMM2 is distributed with a nested directory structure containing the eleven test cases. Each test case is located in a subdirectory (TEST_CASE_1 through TEST_CASE_11) under the parent directory "verification." Several daughter directories are located under each of the test cases. These daughter directories contain input and output files of the test case comparisons as well as notes, plots, and other files as needed for the comparisons. SAMM2 test case output was compared and verified against SAMM1.1, SHARC4.1, or MODTRAN4 as appropriate for the particular test case scenario. If an atmosphere or structure file is needed for a particular run, it is included under the test case directory. These atmospheres were developed for the test cases only and they should be used only for the intended test case.

A sample organizational chart of the directory nesting structure is shown in Diagram 1 and a listing of all the test files are contained in Appendix A. The input files have sufficient information to allow a user to execute SHARC4.1, SAMM1.1, or MODTRAN4 to regenerate the output files. The user should verify that the test case output agrees with his or her own executions. Where there are differences in the comparisons between SAMM2 and the earlier codes, explanations are given in a "notes" file. Generally agreement is excellent but one must be cautious that the comparisons are made with the same spectral resolution (or degraded resolution). The plots are rendered in portable network graphics (.png) compressed format.

Since SHARC4.1, SAMM1.1, and MODTRAN4 have been validated against real-world data, the test case comparisons serve as a secondary validation source for SAMM2. The following sections describe the eleven test cases in detail.
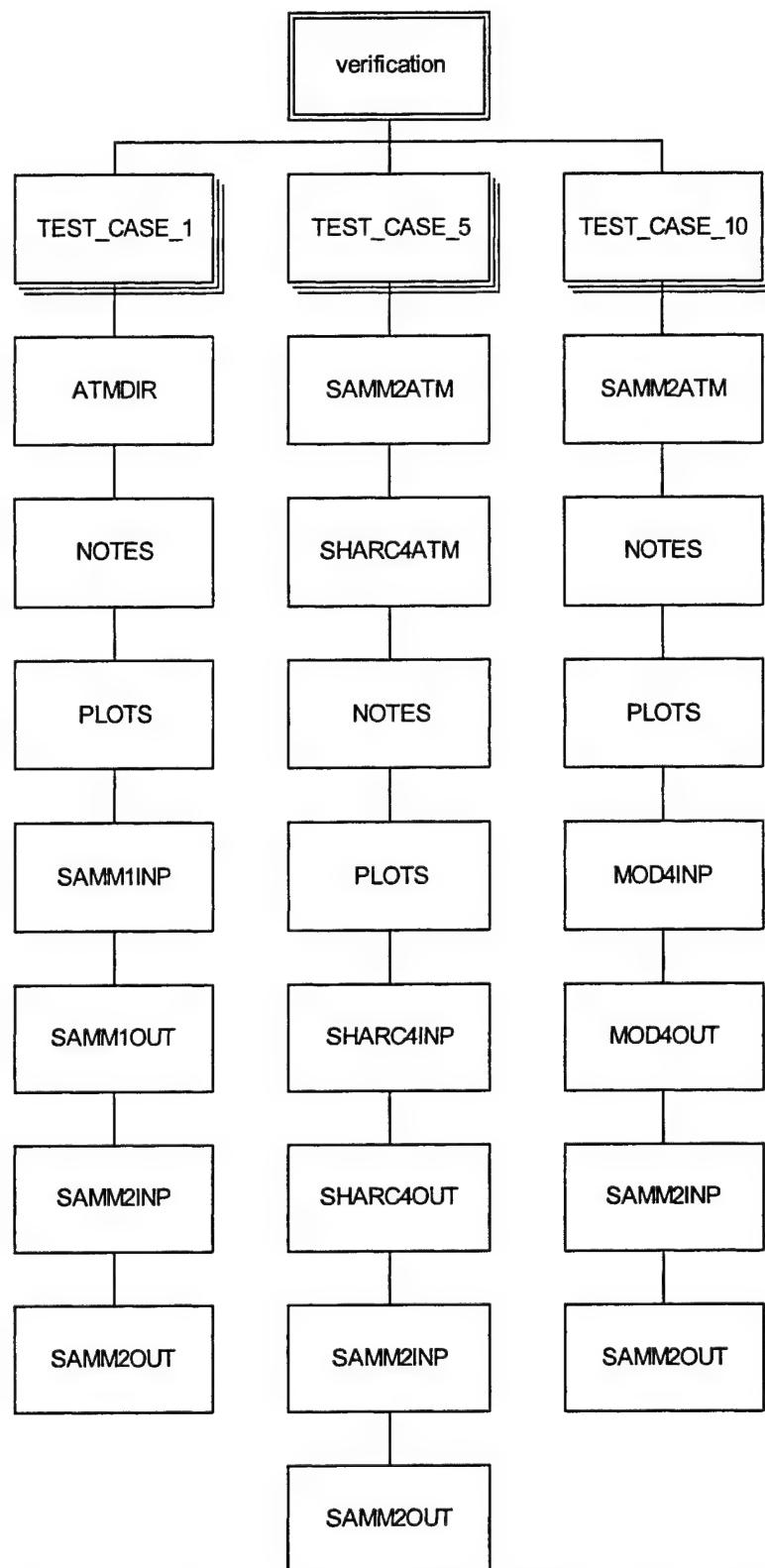
Diagram 1. Sample Organization of Verification Directories

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Preparations

To prepare for running the test cases, the user should first compile and link the several SAMM2 FORTRAN source files and, separately, the INTERPRETER source files (if the chemical kinetics files are changed). On most UNIX systems, just typing "Makesamm2_f90" in the SAMM2 "source" subdirectory will create samm2.exe (the SAMM2 executable). This UNIX script drives a makefile called "Makefile_f90", which is also in the "source" directory. Some users may want to modify this file as this supplied makefile is of the "vanilla" variety, which should work on most systems. It only has the "-O" (optimization) flag for compiling. The source code should be placed in the "source" subdirectory, which also should contain a subdirectory ("objdir_f90") where the source object files are stored upon compilation. In addition, subdirectories "lines", "lines/CONVERT", "popdir", "kindir", "outdir", and "atmdir" should be created. The binary_lines.f program, in the "lines/convert" subdirectory, must be compiled, linked, and used to generate the binary lines file SAMM96.BIN from its ASCII equivalent SAMM96.ASC. The SAMM96.BIN file should then be placed in the "lines" subdirectory. Two additional binary files, LTETAIL.BIN and VOIGTDATA.BIN, required by the line-by-line algorithm in SAMM2, must also be generated from their ASCII equivalents, LTETAIL.ASCII and VOIGTDATA.ASCII. The conversion to binary forms is done by compiling, linking and executing the binary_tail.f and binary_voigtprofile.f programs in the "lines/convert". LTETAIL.BIN contains the Pade approximant coefficients for the extended line tails contributions to the 0.5 cm^{-1} spectral bins processed by the line-by-line algorithm. VOIGTDATA.BIN contains the Voigt profile line shape, the integral under it, and its derivative, tabulated as functions of ε and α, where ε is the ratio of the displacement $\delta\omega$ from the line center to the Lorentz half width γ_L, and α is the ratio of γ_L over the Doppler half width γ_D. All kinetics files should be located in the "kindir" directory. The linking files, if changed from the versions supplied with SAMM2, must be re-created by using the INTERPRETER as explained in Section 7. All atmosphere, atmospheric statistics, solar irradiance, and ground reflectance files should be placed in the "atmdir" subdirectory. The "outdir" subdirectories will initially be empty. The "popdir" subdirectory will initially be empty. If this set of subdirectories is in some way undesirable, the user will need to modify the directory paths in main menu Item 7, as shown in Section 4.2. The INTERPRETER OUTPUT files and the shipped test case files may be placed in any convenient location for comparison with the outputs of the INTERPRETER and SAMM2 itself. Table 1 provides an outline for which files need to be compiled, which executables need to be run, and where to store the various files and databases. Unless changes

are made to the ASCII files that are read, this procedure only needs to be performed once upon installation.

TABLE OF INSTALLATION PROCEDURES			
FORTRAN Files(s)	Create Executables	Result of Execution	Place in Directory
*.f in source directory	samm2_f90.exe (to create, use Makesamm2_f90)	SAMM2 input menu (interactive) SAMM2 execution (batch)	main SAMM2 directory
binary_lines.f	binary_lines.exe	SAMM96.BIN file	lines
binary_tails.f	binary_tails.exe	LTETAIL.BIN file	lines
binary_voigtprofile.f	binary_voigtprofile.exe	VOIGTDATA.BIN file	lines
interp.f	interp.exe (use interp.run for IRIX and interp.bat for PC)	*.CKL files	kindir
Table 1: Installation procedures.			

Running SAMM2

SAMM2 looks for the name(s) of input file(s), for example SAMM2.INP, in the file SAMM2.JOBS. Before starting any SAMM2 run, an input file (or input files for sequential runs) must be listed in the file SAMM2.JOBS. If no input file is listed in SAMM2.JOBS, SAMM2 automatically creates a default input file. This arrangement insures that the user will never lack for an input file upon which to build. Running SAMM2 and immediately exiting should create this default input file. Once a test case input file name is properly listed in SAMM2.JOBS, the user can run the test case and, as for all the cases, compare the output files with those shipped. Many input files may be listed in the SAMM2.JOBS file to enable multiple runs of the code with different input. For Multiple Scattering (MS) runs, an additional data file, named VOD.DAT, will be created in the SAMM2 main directory; this file may be reused for additional runs with the same atmospheric and aerosol/cloud specifications, as described below.

For Multiple Scattering (MS) runs, optical depths, as a function of frequency, for vertical segments are required by the MS algorithm to compute the MS source functions. Once calculated in an initial MS run, these quantities are stored in a file named VOD.DAT to save computing time in the next MS runs if the atmospheric and aerosols/clouds profiles are kept the same, and if the frequency range chosen for those next runs are smaller than the one specified in the initial MS run.

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Before a MS calculation, SAMM2 checks for the existence of the file VOD.DAT, creates one in the main directory if it is not present, then stores in it the vertical optical depths calculated for the specified atmospheric, aerosols/clouds profiles. If a file is present, SAMM2 will check if its atmospheric and aerosols/clouds specifications are consistent with those required by the current run. If they are, the code proceeds by reading the information from this file (skipping the vertical optical depths calculation); otherwise, the existing VOD.DAT is deleted and a new one created to store the vertical optical depths calculated for the new atmospheric, aerosols/clouds profiles. Note that FORTRAN issues a fatal error if the VOD file is empty; in this case, the user should delete the VOD file.

TEST CASE 1

The first case has a nighttime auroral region embedded in an extended ambient region. The selected aurorally enhanced radiators are NO and NO+, and structure calculation is enabled. This case is similar to but not identical to TEST CASE 1 that is distributed with SHARC-3. The TEST1.LOG journal file should be empty, indicating a successful run with no errors or less significant warning or caution messages.

Two plots are included: one for the entire range in wavenumber; the other for an extended section. SAMM1 and SHARC4.1 do not compute the intersection of the line-of-sight with the local region correctly. A new algorithm has been implemented in SAMM2 to correct this problem. However, since the old algorithm can do a good job with a small local region, the results from SAMM1, with a small auroral region, will compare favorably with corresponding results from SAMM2. This caveat in the region size is taken into account in the input files. As shown in Figures D-1 and D-2, spectral agreement is excellent between SAMM2 and SAMM1.1. The percent difference, in band pass radiance is 4.5%. Note that SAMM1.1 was run with a spectral resolution of 1 cm^{-1} and SAMM2 used the internal filter to degrade the SAMM2 spectra to 1 cm^{-1}.

Test Case 1 SAMM1 vs SAMM2
NO and NO+ Two Regions (Auroral)

Figure D-1

Test Case 1 SAMM1 vs SAMM2
NO and NO+ Two Regions (Auroral)
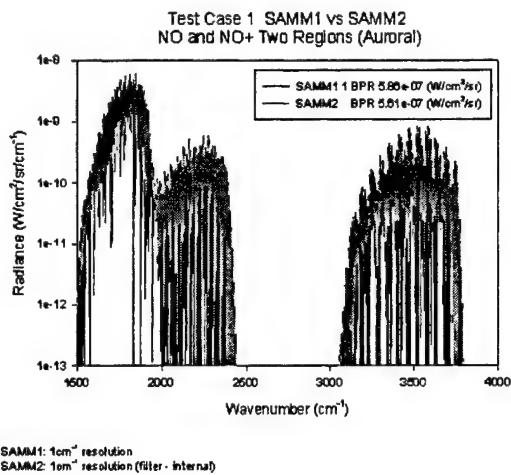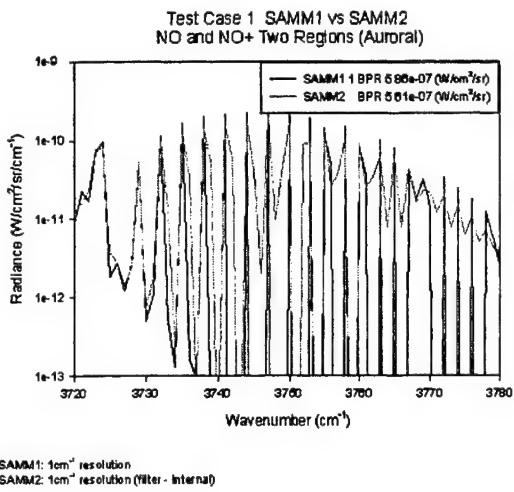
Figure D-2

TEST CASE 2

The second case calculates nighttime emission from all of the supported NLTE radiators (that is, neglecting the MODTRAN LTE species, N2O, NO2, SO2, NH3, HNO3), including the isotopes of CO_2 and H_2O for the limb view. The band pass covers the entire SAMM2 spectral range from 250 to 10000 cm^{-1} (1 to 40 µm). This case is similar to TEST CASE 2 that is distributed with SHARC-3.

Two plots are included: one for the entire range in wavenumber; the other for an extended section. As shown in Figures D-3 and D-4, spectral agreement is excellent between SAMM2 and SAMM1.1. The percent difference, in band pass radiance is 5.4%. Note that SAMM1.1 was run with a spectral resolution of 1 cm^{-1} and SAMM2 used the internal filter to degrade the SAMM2 spectra to 1 cm^{-1}.

Test Case 2 SAMM1 vs SAMM2
CO2, NO, CO, H2O, O3, OH, CH4 - LIMB

Figure D-3

Test Case 2 SAMM1 vs SAMM2
CO2, NO, CO, H2O, O3, OH, CH4 - LIMB

Figure D-4

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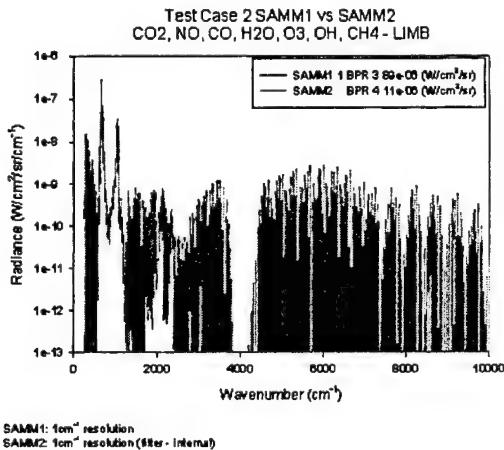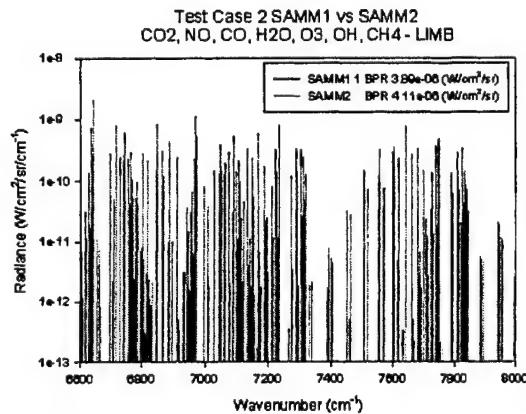
TEST CASE 3

The third test case contains two regions, extended and local aurora. The nighttime aurora has CO_2, NO and NO+ selected as radiators. The line of sight (LOS) is a limb view, starting and ending at the maximum 300 km altitude, capturing radiation from the entire atmosphere above the tangent altitude. This case is similar to TEST CASE 3 that is distributed with SHARC-3.

A series of plots is shown below. Figures D-5 and D-6 compare SAMM1.1 at $1.0\,cm^{-1}$ resolution with SAMM2 at $0.1\,cm^{-1}$ resolution. The spectrum for SAMM2 is the result of using an internal filter to degrade the spectra to $0.1\,cm^{-1}$ resolution. SAMM2 uses an internal triangular slit function with full width at half max equal to the input resolution (in this case $0.1\,cm^{-1}$). The differences that are evident in Figures D-5 and D-6 are due to the SAMM1.1 rectangular equivalent bin width of $1.0\,cm^{-1}$ versus the degraded SAMM2 quasi line-by-line (QBL) spectra. For the spectra in Figures D-5 and D-6, the SAMM2 peaks appear five to ten times greater reflecting the NO doublets, resolved by the SAMM2 QBL algorithm, whose peaks are indeed five to ten times greater.

A more reasonable comparison between codes would be to compute SAMM2 at a high resolution, say $0.1\,cm^{-1}$ and degrade to $1\,cm^{-1}$ using a rectangular slit function. Figures D-7 and D-8 show spectra calculated in this way. This procedure does in fact remove the apparent differences in spectral amplitude (Figures D-7 and D-8). SAMM1.1 however, being a $1.0\,cm^{-1}$ equivalent width code that uses a rectangular bin, cannot distinguish lines that lie in the same spectral bin. The contribution from each line is summed and reported as the spectral radiance at the center (or edge) of the bin. Thus, SAMM1.1 may appear to have spectral features that are narrower than SAMM2 (see Figure D-8), which is correct but misleading. Results from both codes at $1\,cm^{-1}$ resolution show excellent agreement with a percent difference between SAMM2 and SAMM1.1, in integrated bandpass radiance, of -4.2%.

The high spectral resolution capability of the SAMM2 code can be appreciated in Figure D-9 where SAMM2 at $0.1\,cm^{-1}$ resolution is compared with SAMM1.1 at $1.0\,cm^{-1}$ resolution. Clearly, as shown in Figure D-9, the SAMM2 code resolves the emission lines from the S=1/2 and S=3/2 NO individual spin states.
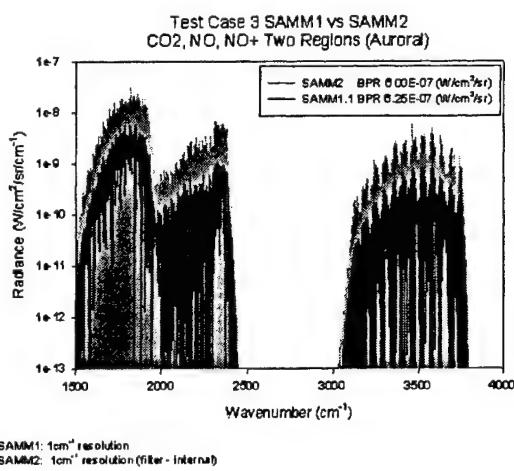
Figure D-5
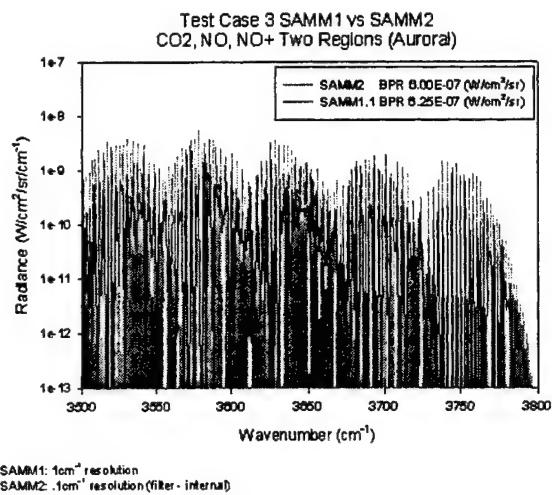
Figure D-6
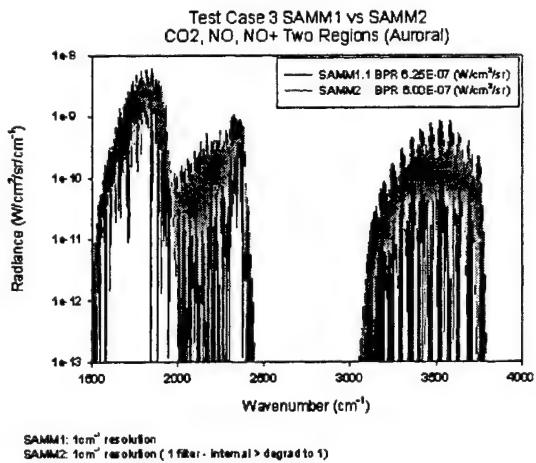
Figure D-7
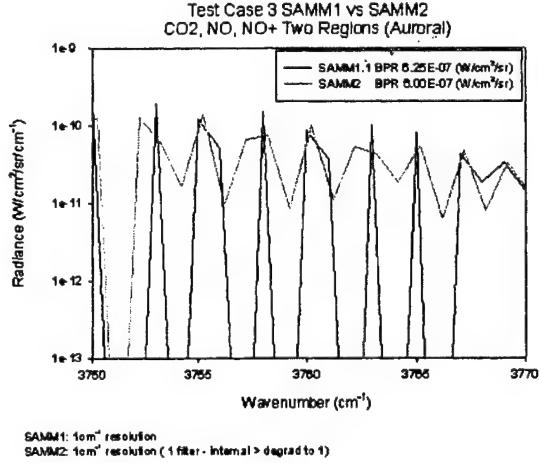
Figure D-8

Figure D-9.

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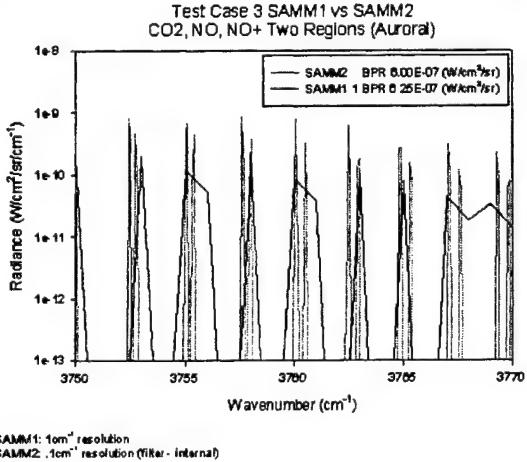
TEST CASE 4

The fourth and fifth test cases demonstrate the use of multiple atmospheric profiles to model the limb terminator. The SHARC Atmosphere Generator (SAG) was used to generate seven files representing solar zenith angles from 91^0 to 102^0, spaced approximately along a line of sight at high latitudes. The atmosphere names follow the rule "T4Z(integer solar zenith angle).ATM" for ease in organizing the case, but no particular rule is required for multiple-profile calculations. The fourth test case calculates the limb terminator radiance of O_3, whose concentration is sensitive to solar illumination. The lines of sight for the first three test cases, discussed thus far, are limb views; the LOS starts and ends at the maximum 300 km altitude, capturing radiation from the entire atmosphere above the tangent altitude. In contrast, this test case uses an observer to space LOS; the observer is located at 184 km and looks downward through the tangent point and back to space (300 km).

Figure D-10 illustrates the comparison between SAMM1.1 at 1.0 cm^{-1} resolution and SAMM2 at 1.0 cm^{-1} resolution (using the internal triangular filter). The agreement is excellent with an integrated bandpass radiance difference, between SAMM2 and SAMM1.1, of 9.4%.

With respect to the small peak at wavenumber 987 cm^{-1}, which results from the 003-002 transition, Rothman's 1998 paper indicates that there are changes to HITRAN around 10 um for the delta ($\nu3$) hot bands. Thus, the SAMM2 line file is different in this spectral region.
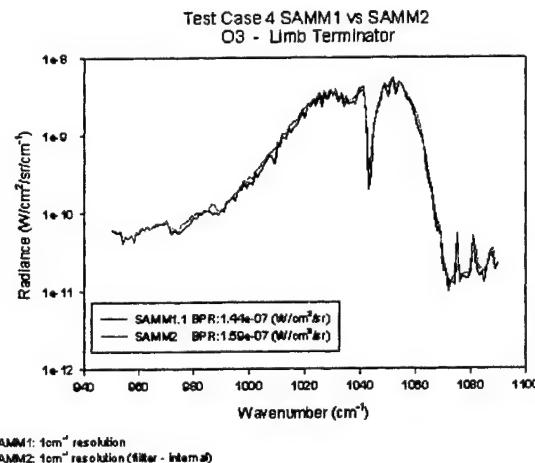

Figure D-10.

TEST CASE 5

The fifth test case again demonstrates the use of multiple atmospheric profiles to model the solar terminator. This test case uses an observer to space LOS; the observer is located at 250 km and looks downward through the tangent point and back to space (300 km). The SHARC Atmosphere Generator (SAG-2) was used to generate seven files representing solar zenith angles from 91^0 to 102^0, spaced approximately along a line of sight at high latitudes. The code calculates the terminator limb radiance of CO2, whose concentration is sensitive to solar illumination. For verification purposes, SAMM2 is compared to SHARC4.1, the high altitude standard radiance code, in Figure D-11. The agreement between SHARC4.1 and SAMM2 is excellent at the same spectral resolution of 1.0 cm^{-1}, with a difference between Samm2 and SHARC4.1, in integrated bandpass radiance, of 5.9%.

Excellent agreement is obtained except in the region greater than 2350 cm^{-1}. This is due to a binning artifact in SHARC4.1. The SAMM2 results are correct.

Test Case 5 SHARC4.1 vs SAMM2
CO2 Terminator

SHARC4.1: 1cm^{-1} resolution
SAMM2: 1cm^{-1} resolution (filter - internal)

Figure D-11.

TEST CASE 6

This test case demonstrates the SAMM2 structure capability with CO_2 as the radiator. The narrow (100 cm^{-1}) spectral range considered is near the center of the CO_2 4.3 μm band. The volume emission and variance distribution output files, TEST6.VMIS and TEST6.VDIS, contain the radiance contribution function and the radiance variance distribution function for each segment along the LOS. The latter function is a measure of each LOS segment contribution to the radiance structure. This test case is similar to TEST CASE 1 that is distributed with SHARC4.1. Excellent agreement is obtained between SAMM2 and SHARC4.1 volume emissions, shown as a function of LOS segments in Figure D-12a. For this optically thick band, it can be seen that most of the radiance comes from the near side of the tangent point of the limb view. The SAMM2 variance distribution shown in Figure D-12b indicates disagreement with SHARC4.1 in the near side region of the tangent point. Our validation work showed that the SAMM2 calculation is the correct one; the disagreement
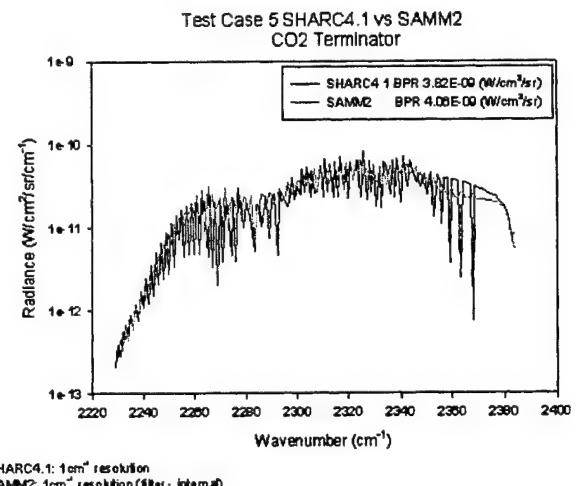
is caused by a temperature derivative term that could not be implemented for the Equivalent Width (EW) formalism used in SHARC4.1. The LBL formalism used in SAMM2 allows all temperature derivative terms to be correctly implemented. Figure D-12c shows that the (incorrect) SHARC4.1 results are obtained when this derivative term is left out of the SAMM2 calculations. The difference in the relative standard deviation and the differences in the correlation lengths in the .2D files are also due to the temperature derivative term that was not implemented in SHARC4.1. Note that in Figures D-12a-D-12c, the SAMM2 and SHARC4.1 results are labeled as LBL and EW, respectively.

The percent difference, in bandpass radiance between SAMM2 and SHARC4.1 is 0.99%.
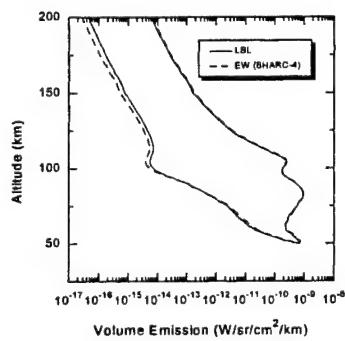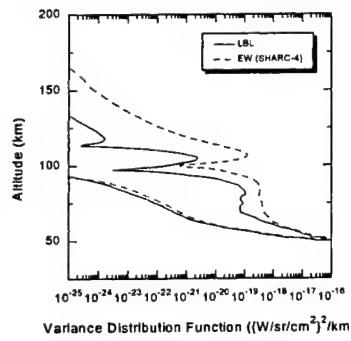
| Figure D-12a | Figure D-12b | Figure D-12c |
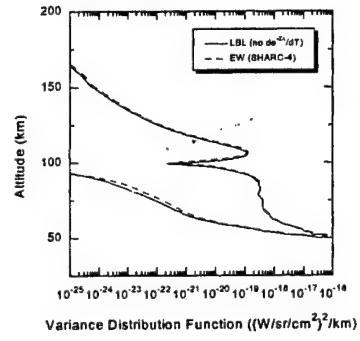
TEST CASE 7

The seventh test case is a multiple lines-of-sight calculation looking down to an altitude of 30 km from space in the CO_2 band 2250-2350 cm^{-1}, producing .2D and .3D structure files that can be used later for scene generation by the AFRL SAMM2 Scene Generation tool, SIG (SHARC Image Generator). Also produced are the numerical radiance covariance vs. lag angle (.COVA file) and lag distance (.COVD file), modified Bessel function approximation for the radiance covariance, and the radiance variance distribution function (.VDIS file). This test case is similar to TEST CASE 2 that is distributed with SHARC4.1. The agreement between SAMM2 and SHARC4.1 is excellent with a difference in integrated band pass radiance for the zenith angles, 120^0, 122^0, and 124^0 of -1.7%, -1.0%, and -1.8% respectively.

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Note that because the spectral range is only 100 cm⁻¹, (2250 – 2350), and the resolution is 50 cm⁻¹, the code gives only one value for the spectrum at 2300 cm⁻¹. Recall that the specified resolution is full width at half max. A data point at 2300 cm⁻¹ corresponds to the triangular slit function centered at 2300 cm⁻¹. Its full width spans 2250 – 2350, i.e., the entire range in which the radiative transfer problem is being calculated. To get values at the beginning and end of the spectrum, the range of the spectral calculation would have to be expanded by introducing a wing value equal to the desired resolution.

TEST CASE 8

The eighth test case is a limb view with multiple lines-of-sight test, producing .2D, .3D, and covariance structure files that can be used later for scene generation by the AFRL SAMM2 Scene Generation tool, SIG (SHARC Image Generator). All NLTE radiators are included and the spectral range covers from 900 to 1700 cm-1, including the ozone 9.6 µm band.

Three comparisons at 50 km, 70 km, and 90 km tangent altitudes are shown in Figures D-13-D-15 below. The differences, in bandpass radiance between SAMM2 and SHARC4.1 for these tangent heights are -.70%, -15.6%, and –2.1%, respectively. Changes in the line file account for differences in the spectral region between 900 – 1000 cm-1.

Figure D-13.

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Test Case 8 SHARC4.1 vs SAMM2
Narrow MWIR Band - UMB Structure, Multiple LOS

Figure D-14.

SHARC4 1: 1cm⁻¹ resolution
SAMM2: 1cm⁻¹ resolution (filter - internal)

Test Case 8 SHARC4.1 vs SAMM2
Narrow MWIR Band - UMB Structure, Multiple LOS

Figure D-15.

SHARC4.1: 1cm⁻¹ resolution
SAMM2: 1cm⁻¹ resolution (filter - internal)
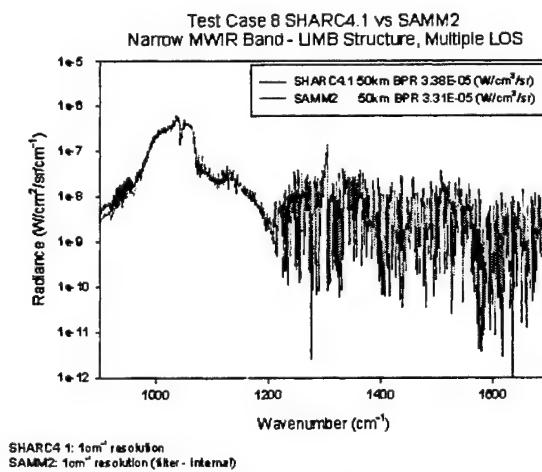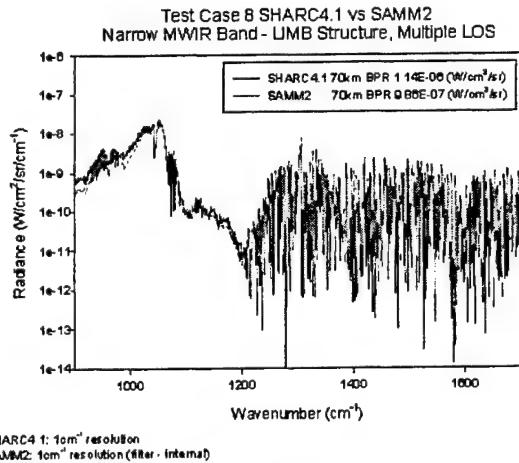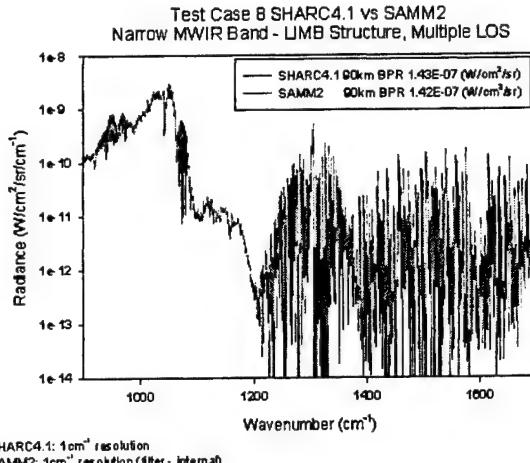
TEST CASE 9

The ninth test case is a test of the Multiple Scattering (MS) capability of SAMM2. For validation purposes, SAMM2 is being compared to MODTRAN4 as these codes have an updated cloud extinction coefficient database not included in SAMM1.1.

TEST CASE 9 performs a nadir view from 100 km with the important SHARC and MODTRAN radiators in the 3000 to 5000 cm-1 spectral region, including clouds and aerosols. The ground albedo is set to 0.5. This test illustrates the strong MS contribution from 4000 to 5000 cm-1. The agreement between MODTRAN4 and SAMM2, shown in Figure D-16, is very good with a percent difference in integrated band radiance of 3.0%. The disagreement in the 3500-3800 cm-1 region was found to be due to problems in MODTRAN4 that are being corrected at the time this report is prepared. The corrections to


Test Case 9 MODTRAN4 vs SAMM2
100km - 0km, Clouds/Aerosols Ground Albedo = 0.5

MOD4: 1cm⁻¹ resolution
SAMM2: 1cm⁻¹ resolution (filter - internal)
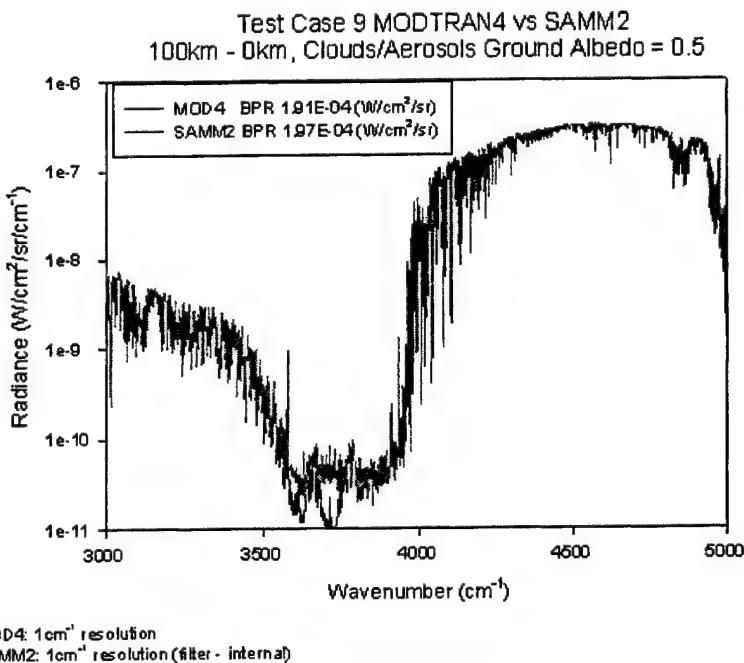
Figure D-16.

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MODTRAN are expected to eliminate any remaining disagreement. It should be emphasized the agreement seen is not simply a result of any common algorithm between the two codes. The methods used to compute the radiance in the two codes are different. Unlike MODTRAN, which uses the Planck Function for all molecular emission sources, the SAMM2 source functions at all altitudes are obtained from a chemical kinetic model (CHEMKIN). At low altitudes, where LTE conditions apply, these source functions reduce the NLTE source to a Blackbody Function. In addition, instead of band model values, the SAMM2 spectral radiances are produced by combining the just mentioned source functions with true line by line data, and line broadening parameters, read directly from the HITRAN compilation. For this test case, it should be pointed out that the ground albedo value does not affect the radiance because of the presence of clouds (i.e., the same observed radiance would be obtained for a zero ground albedo). In TEST CASES 10 and 11 below, the effect of ground reflectance will be illustrated.

TEST CASES 10 and 11

The tenth and eleventh test cases are tests of the Multiple Scattering (MS) capability of SAMM2. These low altitude scenarios test the full multiple scattering capability, including the ground reflectance terms and the relayering algorithm for low altitudes. TEST CASE 10 performs a nadir view from 2 km with the important SHARC and MODTRAN radiators in the 3000 to 5000 cm^{-1} spectral region, including aerosols, but not clouds. The ground albedo is set to zero. TEST CASE 11 is identical except with a ground albedo of 0.5. Both of these tests illustrate the strong MS contribution from 4000 to 5000 cm^{-1}. For TEST CASE 11, there is, in addition, a strong enhancement from ground reflectance. The agreement between MODTRAN4 and SAMM2, shown in Figure D-17 for TEST CASE 10, is good with a percent difference of -19%. The displacement between $3500 - 4000 \ cm^{-1}$ is probably due to a slight temperature difference. The one between 4000 $- 4500 \ cm^{-1}$ may be due to the slight differences between the multiple scattering contributions between the two codes. The multiple scattering algorithms use the layer optical depths as inputs. In SAMM2, these values are line-by-line values at particular frequencies, whereas, in MODTRAN4 these values are band model (averaged) values. So slight differences in the multiple scattering solutions are unavoidable. In general, had the multiple scattering solutions been obtained at .001 cm^{-1} resolution, then the SAMM2 results would be the most accurate ones. However, multiple scattering

contributions were gotten at 1 cm^{-1} resolution, and interpolation was used to generate the data in between. In Figure D-18 the region, 4000 – 4150 cm^{-1}, shows the effect of the ground albedo where the radiance is dominated by the ground reflectance terms. The percent difference in integrated band radiance for TEST CASE 11 is 5.6%. The agreement is excellent between MODTRAN4 and SAMM2.
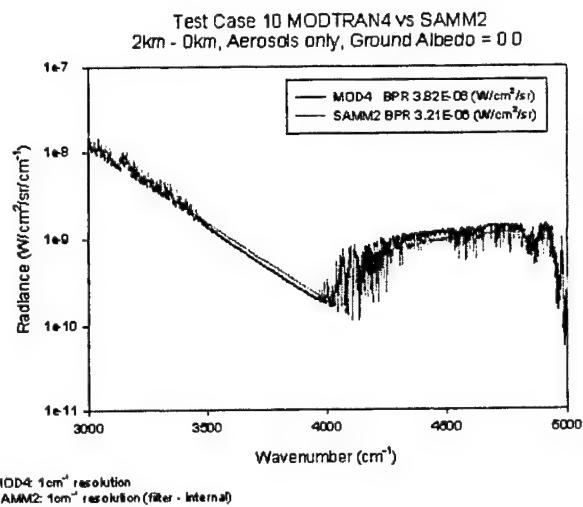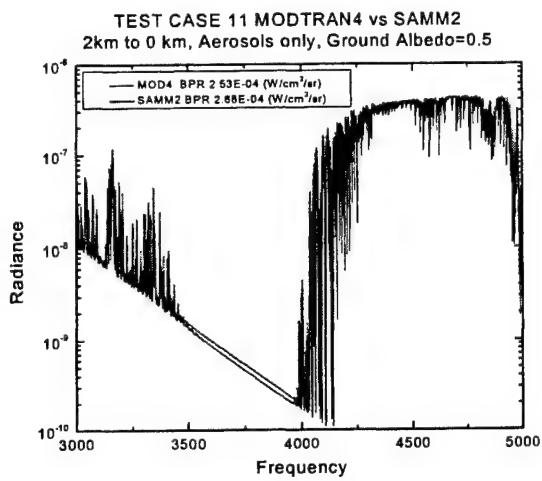

Figure D-17.

Figure D-18.

APPENDIX E
SAMM2 HIGH-LATITUDE NIGHT ATMOSPHERIC PROFILE

ATMOSPHERE NAME (SAMM2 TEST CASE - HIGH LAT SUMMER NIGHT)
NIG65N.ATM
END
NUMBER OF LAYERS
103
END
DAY-NIGHT VARIABLE AND EXOATMOSPHERIC TEMPERATURE
 NIGHT   1028.21
END
SPECIES
O2 O CO2 N2 NO O3 H OH CO H2O CH4 HNO3 N2O NH3 NO2 SO2
END
ALTITUDES
```
   0.00    1.00    2.00    3.00    4.00
   5.00    6.00    7.00    8.00    9.00
  10.00   11.00   12.00   13.00   14.00
  15.00   16.00   17.00   18.00   19.00
  20.00   21.00   22.00   23.00   24.00
  26.00   28.00   30.00   32.00   34.00
  36.00   38.00   40.00   42.00   44.00
  46.00   48.00   50.00   52.00   54.00
  56.00   58.00   60.00   62.00   64.00
  66.00   68.00   70.00   72.00   74.00
  76.00   78.00   80.00   82.00   84.00
  86.00   88.00   90.00   92.00   94.00
  96.00   98.00  100.00  102.00  104.00
 106.00  108.00  110.00  112.00  114.00
 116.00  118.00  120.00  122.00  124.00
 126.00  128.00  130.00  132.00  134.00
 136.00  138.00  140.00  142.00  144.00
 146.00  148.00  150.00  160.00  170.00
 180.00  190.00  200.00  210.00  220.00
 230.00  240.00  250.00  260.00  270.00
 280.00  290.00  300.00
```
END
TEMPERATURES
```
0.2807E+03 0.2770E+03 0.2718E+03 0.2655E+03 0.2588E+03
0.2520E+03 0.2455E+03 0.2394E+03 0.2342E+03 0.2299E+03
0.2267E+03 0.2246E+03 0.2236E+03 0.2232E+03 0.2231E+03
0.2232E+03 0.2231E+03 0.2229E+03 0.2227E+03 0.2224E+03
0.2222E+03 0.2221E+03 0.2221E+03 0.2222E+03 0.2224E+03
0.2233E+03 0.2248E+03 0.2271E+03 0.2302E+03 0.2344E+03
0.2395E+03 0.2450E+03 0.2506E+03 0.2559E+03 0.2603E+03
0.2633E+03 0.2646E+03 0.2645E+03 0.2630E+03 0.2604E+03
```

```
 0.2570E+03 0.2529E+03 0.2483E+03 0.2432E+03 0.2377E+03
 0.2319E+03 0.2260E+03 0.2199E+03 0.2138E+03 0.2074E+03
 0.2003E+03 0.1933E+03 0.1867E+03 0.1810E+03 0.1764E+03
 0.1731E+03 0.1714E+03 0.1716E+03 0.1738E+03 0.1780E+03
 0.1838E+03 0.1911E+03 0.1994E+03 0.2084E+03 0.2184E+03
 0.2297E+03 0.2428E+03 0.2583E+03 0.2772E+03 0.2998E+03
 0.3262E+03 0.3559E+03 0.3881E+03 0.4207E+03 0.4510E+03
 0.4795E+03 0.5066E+03 0.5323E+03 0.5568E+03 0.5801E+03
 0.6021E+03 0.6231E+03 0.6431E+03 0.6620E+03 0.6800E+03
 0.6971E+03 0.7134E+03 0.7288E+03 0.7953E+03 0.8469E+03
 0.8869E+03 0.9181E+03 0.9423E+03 0.9611E+03 0.9758E+03
 0.9872E+03 0.9961E+03 0.1003E+04 0.1009E+04 0.1013E+04
 0.1016E+04 0.1019E+04 0.1021E+04
END
N2 DENSITIES
 0.2043E+20 0.1831E+20 0.1648E+20 0.1485E+20 0.1338E+20
 0.1202E+20 0.1075E+20 0.9577E+19 0.8478E+19 0.7455E+19
 0.6511E+19 0.5648E+19 0.4874E+19 0.4192E+19 0.3600E+19
 0.3089E+19 0.2653E+19 0.2280E+19 0.1959E+19 0.1683E+19
 0.1446E+19 0.1241E+19 0.1065E+19 0.9140E+18 0.7837E+18
 0.5756E+18 0.4223E+18 0.3096E+18 0.2270E+18 0.1666E+18
 0.1226E+18 0.9063E+17 0.6745E+17 0.5059E+17 0.3829E+17
 0.2926E+17 0.2256E+17 0.1750E+17 0.1363E+17 0.1065E+17
 0.8321E+16 0.6496E+16 0.5062E+16 0.3933E+16 0.3044E+16
 0.2345E+16 0.1796E+16 0.1367E+16 0.1033E+16 0.7754E+15
 0.5784E+15 0.4271E+15 0.3113E+15 0.2235E+15 0.1580E+15
 0.1101E+15 0.7562E+14 0.5135E+14 0.3458E+14 0.2323E+14
 0.1565E+14 0.1063E+14 0.7294E+13 0.5075E+13 0.3576E+13
 0.2549E+13 0.1836E+13 0.1334E+13 0.9780E+12 0.7239E+12
 0.5422E+12 0.4118E+12 0.3180E+12 0.2505E+12 0.2019E+12
 0.1656E+12 0.1378E+12 0.1160E+12 0.9866E+11 0.8469E+11
 0.7328E+11 0.6385E+11 0.5597E+11 0.4934E+11 0.4371E+11
 0.3889E+11 0.3475E+11 0.3116E+11 0.1888E+11 0.1210E+11
 0.8048E+10 0.5502E+10 0.3836E+10 0.2714E+10 0.1942E+10
 0.1402E+10 0.1019E+10 0.7443E+09 0.5462E+09 0.4023E+09
 0.2971E+09 0.2200E+09 0.1633E+09
END
O2 DENSITIES
 0.5481E+19 0.4913E+19 0.4421E+19 0.3984E+19 0.3588E+19
 0.3224E+19 0.2885E+19 0.2569E+19 0.2274E+19 0.2000E+19
 0.1747E+19 0.1515E+19 0.1308E+19 0.1125E+19 0.9657E+18
 0.8288E+18 0.7118E+18 0.6115E+18 0.5255E+18 0.4516E+18
 0.3879E+18 0.3331E+18 0.2858E+18 0.2452E+18 0.2102E+18
 0.1544E+18 0.1133E+18 0.8307E+17 0.6091E+17 0.4469E+17
 0.3288E+17 0.2431E+17 0.1809E+17 0.1357E+17 0.1027E+17
```

0.7850E+16 0.6051E+16 0.4694E+16 0.3658E+16 0.2857E+16
0.2232E+16 0.1743E+16 0.1358E+16 0.1055E+16 0.8162E+15
0.6284E+15 0.4811E+15 0.3660E+15 0.2764E+15 0.2072E+15
0.1544E+15 0.1138E+15 0.8279E+14 0.5928E+14 0.4175E+14
0.2893E+14 0.1973E+14 0.1328E+14 0.8828E+13 0.5835E+13
0.3852E+13 0.2549E+13 0.1697E+13 0.1139E+13 0.7699E+12
0.5238E+12 0.3584E+12 0.2466E+12 0.1708E+12 0.1193E+12
0.8439E+11 0.6066E+11 0.4448E+11 0.3340E+11 0.2577E+11
0.2032E+11 0.1632E+11 0.1332E+11 0.1102E+11 0.9222E+10
0.7801E+10 0.6659E+10 0.5730E+10 0.4964E+10 0.4328E+10
0.3793E+10 0.3341E+10 0.2955E+10 0.1685E+10 0.1022E+10
0.6458E+09 0.4203E+09 0.2794E+09 0.1888E+09 0.1291E+09
0.8907E+08 0.6192E+08 0.4330E+08 0.3043E+08 0.2146E+08
0.1519E+08 0.1078E+08 0.7667E+07
END
O DENSITIES
0.6090E+00 0.6090E+00 0.6090E+00 0.6090E+00 0.6090E+00
0.6090E+00 0.6090E+00 0.6090E+00 0.6090E+00 0.6090E+00
0.6090E+00 0.6090E+00 0.6090E+00 0.6090E+00 0.6090E+00
0.6090E+00 0.6090E+00 0.6090E+00 0.6090E+00 0.6090E+00
0.6090E+00 0.6090E+00 0.6090E+00 0.6090E+00 0.6090E+00
0.6090E+00 0.6090E+00 0.6090E+00 0.6090E+00 0.6090E+00
0.6090E+00 0.6090E+00 0.6090E+00 0.6090E+00 0.6090E+00
0.6090E+00 0.6090E+00 0.6090E+00 0.6090E+00 0.6090E+00
0.6090E+00 0.6090E+00 0.6090E+00 0.6090E+01 0.6090E+02
0.6090E+03 0.6090E+04 0.6090E+05 0.6090E+06 0.5481E+07
0.4872E+08 0.4263E+09 0.3654E+10 0.1096E+11 0.2862E+11
0.6090E+11 0.1067E+12 0.1600E+12 0.2093E+12 0.2447E+12
0.2616E+12 0.2612E+12 0.2480E+12 0.2271E+12 0.2026E+12
0.1772E+12 0.1527E+12 0.1299E+12 0.1095E+12 0.9173E+11
0.7663E+11 0.6407E+11 0.5385E+11 0.4572E+11 0.3940E+11
0.3432E+11 0.3015E+11 0.2670E+11 0.2380E+11 0.2133E+11
0.1923E+11 0.1741E+11 0.1583E+11 0.1446E+11 0.1325E+11
0.1218E+11 0.1123E+11 0.1038E+11 0.7256E+10 0.5303E+10
0.4000E+10 0.3090E+10 0.2429E+10 0.1937E+10 0.1561E+10
0.1270E+10 0.1040E+10 0.8573E+09 0.7098E+09 0.5901E+09
0.4923E+09 0.4118E+09 0.3456E+09
END
CO2 DENSITIES
0.8896E+16 0.7975E+16 0.7176E+16 0.6467E+16 0.5824E+16
0.5233E+16 0.4683E+16 0.4170E+16 0.3691E+16 0.3246E+16
0.2835E+16 0.2459E+16 0.2122E+16 0.1825E+16 0.1567E+16
0.1345E+16 0.1155E+16 0.9926E+15 0.8530E+15 0.7329E+15
0.6296E+15 0.5406E+15 0.4639E+15 0.3980E+15 0.3412E+15
0.2506E+15 0.1839E+15 0.1348E+15 0.9886E+14 0.7254E+14

0.5338E+14 0.3946E+14 0.2937E+14 0.2203E+14 0.1667E+14
0.1274E+14 0.9821E+13 0.7619E+13 0.5937E+13 0.4637E+13
0.3623E+13 0.2829E+13 0.2204E+13 0.1712E+13 0.1326E+13
0.1023E+13 0.7845E+12 0.5977E+12 0.4521E+12 0.3395E+12
0.2532E+12 0.1869E+12 0.1361E+12 0.9760E+11 0.6882E+11
0.4773E+11 0.3258E+11 0.2191E+11 0.1375E+11 0.8559E+10
0.5311E+10 0.3297E+10 0.2054E+10 0.1287E+10 0.8113E+09
0.5144E+09 0.3281E+09 0.2106E+09 0.1362E+09 0.8910E+08
0.5910E+08 0.3988E+08 0.2747E+08 0.2031E+08 0.1541E+08
0.1193E+08 0.9390E+07 0.7495E+07 0.6055E+07 0.4943E+07
0.4073E+07 0.3384E+07 0.2831E+07 0.2384E+07 0.2019E+07
0.1719E+07 0.1470E+07 0.1262E+07 0.6207E+06 0.3253E+06
0.1781E+06 0.1007E+06 0.5826E+05 0.3431E+05 0.2049E+05
0.1236E+05 0.7522E+04 0.4611E+04 0.2840E+04 0.1757E+04
0.1091E+04 0.6800E+03 0.4249E+03
END
H DENSITIES
0.1000E-04 0.1000E-04 0.1000E-04 0.1000E-04 0.1000E-04
0.1000E-04 0.1000E-04 0.1000E-04 0.1000E-04 0.1000E-04
0.1000E-04 0.1000E-04 0.1000E-04 0.1000E-04 0.1000E-04
0.1000E-04 0.1000E-04 0.1000E-04 0.1000E-04 0.1000E-04
0.1000E-04 0.1000E-04 0.1000E-04 0.1000E-04 0.1000E-04
0.1000E-04 0.1000E-04 0.1000E-04 0.1000E-04 0.1000E-04
0.1000E-04 0.1000E-04 0.1000E-04 0.1000E-04 0.1000E-04
0.1000E-04 0.1000E-04 0.1000E-04 0.1000E-04 0.1000E-04
0.1000E-04 0.1000E-04 0.1000E-04 0.1000E-04 0.1000E-04
0.1000E-04 0.1000E-04 0.1000E-04 0.1000E-04 0.1363E+05
0.3679E+06 0.8858E+07 0.6204E+08 0.1348E+09 0.1515E+09
0.1268E+09 0.9450E+08 0.6782E+08 0.4861E+08 0.3547E+08
0.2660E+08 0.2054E+08 0.1631E+08 0.1326E+08 0.1098E+08
0.9198E+07 0.7765E+07 0.6577E+07 0.5572E+07 0.4717E+07
0.3990E+07 0.3377E+07 0.2864E+07 0.2442E+07 0.2099E+07
0.1816E+07 0.1579E+07 0.1381E+07 0.1212E+07 0.1070E+07
0.9481E+06 0.8440E+06 0.7547E+06 0.6779E+06 0.6116E+06
0.5542E+06 0.5045E+06 0.4611E+06 0.3135E+06 0.2345E+06
0.1895E+06 0.1627E+06 0.1458E+06 0.1348E+06 0.1274E+06
0.1221E+06 0.1182E+06 0.1152E+06 0.1128E+06 0.1109E+06
0.1091E+06 0.1076E+06 0.1062E+06
END
NO DENSITIES
0.7847E+10 0.7034E+10 0.6329E+10 0.5704E+10 0.5137E+10
0.4615E+10 0.4131E+10 0.3678E+10 0.3256E+10 0.2863E+10
0.2501E+10 0.2169E+10 0.1872E+10 0.1605E+10 0.1359E+10
0.1119E+10 0.9103E+09 0.7354E+09 0.6019E+09 0.5258E+09
0.4720E+09 0.4403E+09 0.4188E+09 0.4212E+09 0.4525E+09

0.6482E+09 0.7880E+09 0.9712E+09 0.1164E+10 0.1269E+10
0.1248E+10 0.1124E+10 0.9671E+09 0.7615E+09 0.5775E+09
0.4276E+09 0.3135E+09 0.2307E+09 0.1784E+09 0.1382E+09
0.1076E+09 0.8400E+08 0.6545E+08 0.5125E+08 0.3998E+08
0.3160E+08 0.2530E+08 0.2012E+08 0.1739E+08 0.1493E+08
0.1319E+08 0.1194E+08 0.1066E+08 0.1124E+08 0.1166E+08
0.1228E+08 0.1314E+08 0.1389E+08 0.1621E+08 0.1892E+08
0.2208E+08 0.2577E+08 0.3007E+08 0.3550E+08 0.3884E+08
0.4051E+08 0.4135E+08 0.4177E+08 0.4093E+08 0.3968E+08
0.3759E+08 0.3508E+08 0.3174E+08 0.2757E+08 0.2381E+08
0.2088E+08 0.1838E+08 0.1629E+08 0.1462E+08 0.1337E+08
0.1232E+08 0.1136E+08 0.1044E+08 0.9640E+07 0.8916E+07
0.8229E+07 0.7622E+07 0.7053E+07 0.5018E+07 0.3570E+07
0.2538E+07 0.1776E+07 0.1243E+07 0.8695E+06 0.6083E+06
0.4256E+06 0.2978E+06 0.2084E+06 0.1458E+06 0.1020E+06
0.7137E+05 0.4994E+05 0.3494E+05
END
O3 DENSITIES
0.8728E+12 0.9411E+12 0.1019E+13 0.9912E+12 0.9640E+12
0.9007E+12 0.8383E+12 0.8336E+12 0.8240E+12 0.8316E+12
0.8335E+12 0.1077E+13 0.1386E+13 0.1694E+13 0.2067E+13
0.2406E+13 0.2803E+13 0.3080E+13 0.3384E+13 0.3585E+13
0.3796E+13 0.3795E+13 0.3793E+13 0.3784E+13 0.3774E+13
0.3156E+13 0.2601E+13 0.2143E+13 0.1712E+13 0.1370E+13
0.1048E+13 0.7690E+12 0.5679E+12 0.3684E+12 0.2412E+12
0.1583E+12 0.1038E+12 0.6832E+11 0.4664E+11 0.3183E+11
0.2257E+11 0.1643E+11 0.1178E+11 0.9645E+10 0.7356E+10
0.5726E+10 0.4375E+10 0.3124E+10 0.2023E+10 0.1322E+10
0.8636E+09 0.5643E+09 0.3687E+09 0.3094E+09 0.4121E+09
0.5616E+09 0.6566E+09 0.6280E+09 0.4829E+09 0.3062E+09
0.1665E+09 0.8107E+08 0.3699E+08 0.1649E+08 0.7300E+07
0.3221E+07 0.1410E+07 0.6054E+06 0.2532E+06 0.1046E+06
0.4361E+05 0.1884E+05 0.8655E+04 0.4345E+04 0.2428E+04
0.1464E+04 0.9369E+03 0.6293E+03 0.4399E+03 0.3179E+03
0.2364E+03 0.1800E+03 0.1399E+03 0.1106E+03 0.8887E+02
0.7234E+02 0.5959E+02 0.4960E+02 0.2235E+02 0.1158E+02
0.5469E+01 0.2506E+01 0.1046E+01 0.3174E+00 0.1504E+00
0.8642E-01 0.5022E-01 0.2943E-01 0.1737E-01 0.1031E-01
0.6149E-02 0.3681E-02 0.2213E-02
END
OH DENSITIES
0.1151E+07 0.1032E+07 0.9283E+06 0.8366E+06 0.7534E+06
0.6769E+06 0.6058E+06 0.5407E+06 0.4830E+06 0.4352E+06
0.3901E+06 0.3471E+06 0.3083E+06 0.2786E+06 0.2604E+06
0.2670E+06 0.2802E+06 0.3035E+06 0.3260E+06 0.3534E+06

0.3998E+06 0.5404E+06 0.6943E+06 0.8881E+06 0.1164E+07
0.2239E+07 0.3204E+07 0.4638E+07 0.7984E+07 0.1243E+08
0.1741E+08 0.2187E+08 0.2461E+08 0.2450E+08 0.2285E+08
0.2012E+08 0.1724E+08 0.1512E+08 0.1353E+08 0.1213E+08
0.1148E+08 0.1145E+08 0.1141E+08 0.1198E+08 0.1253E+08
0.1279E+08 0.1273E+08 0.1258E+08 0.1135E+08 0.9553E+07
0.8043E+07 0.6771E+07 0.5700E+07 0.3256E+07 0.1772E+07
0.9140E+06 0.4451E+06 0.2042E+06 0.8840E+05 0.3675E+05
0.1495E+05 0.6068E+04 0.2506E+04 0.1074E+04 0.4777E+03
0.2191E+03 0.1023E+03 0.4783E+02 0.2213E+02 0.1019E+02
0.4748E+01 0.2279E+01 0.1150E+01 0.6231E+00 0.3680E+00
0.2312E+00 0.1525E+00 0.1047E+00 0.7432E-01 0.5426E-01
0.4059E-01 0.3101E-01 0.2413E-01 0.1908E-01 0.1531E-01
0.1245E-01 0.1024E-01 0.8523E-02 0.3893E-02 0.2122E-02
0.1095E-02 0.5653E-03 0.2718E-03 0.9638E-04 0.5380E-04
0.3660E-04 0.2522E-04 0.1753E-04 0.1226E-04 0.8614E-05
0.6070E-05 0.4288E-05 0.3034E-05
END
CO DENSITIES
0.2877E+13 0.2571E+13 0.2303E+13 0.2069E+13 0.1852E+13
0.1664E+13 0.1484E+13 0.1318E+13 0.1161E+13 0.1019E+13
0.8860E+12 0.7637E+12 0.6548E+12 0.5462E+12 0.4520E+12
0.3529E+12 0.2718E+12 0.1984E+12 0.1403E+12 0.1113E+12
0.8729E+11 0.6915E+11 0.5457E+11 0.4313E+11 0.3382E+11
0.2124E+11 0.1336E+11 0.8163E+10 0.5175E+10 0.3202E+10
0.2141E+10 0.1588E+10 0.1186E+10 0.1042E+10 0.9038E+09
0.8828E+09 0.9087E+09 0.8821E+09 0.1026E+10 0.1066E+10
0.1146E+10 0.1222E+10 0.1207E+10 0.1280E+10 0.1256E+10
0.1215E+10 0.1153E+10 0.1046E+10 0.9944E+09 0.8990E+09
0.8453E+09 0.7979E+09 0.7079E+09 0.6814E+09 0.6040E+09
0.5230E+09 0.4416E+09 0.3556E+09 0.2960E+09 0.2368E+09
0.1911E+09 0.1551E+09 0.1240E+09 0.1005E+09 0.8088E+08
0.6451E+08 0.5116E+08 0.4063E+08 0.3183E+08 0.2510E+08
0.1982E+08 0.1572E+08 0.1267E+08 0.1003E+08 0.8124E+07
0.6698E+07 0.5602E+07 0.4742E+07 0.4057E+07 0.3503E+07
0.3048E+07 0.2671E+07 0.2356E+07 0.2089E+07 0.1861E+07
0.1666E+07 0.1498E+07 0.1351E+07 0.8446E+06 0.5590E+06
0.3851E+06 0.2734E+06 0.1985E+06 0.1468E+06 0.1101E+06
0.8370E+05 0.6430E+05 0.4986E+05 0.3899E+05 0.3073E+05
0.2439E+05 0.1948E+05 0.1565E+05
END
H2O DENSITIES
0.2005E+18 0.1455E+18 0.9364E+17 0.5467E+17 0.2964E+17
0.1528E+17 0.7668E+16 0.3831E+16 0.1948E+16 0.1305E+16
0.8688E+15 0.5743E+15 0.3777E+15 0.2476E+15 0.1620E+15

0.1060E+15 0.6935E+14 0.4541E+14 0.2974E+14 0.1947E+14
0.1275E+14 0.8342E+13 0.5456E+13 0.4740E+13 0.4116E+13
0.3101E+13 0.2333E+13 0.1755E+13 0.1320E+13 0.9932E+12
0.7496E+12 0.5685E+12 0.4339E+12 0.3319E+12 0.2547E+12
0.1961E+12 0.1515E+12 0.1171E+12 0.9033E+11 0.6987E+11
0.5356E+11 0.4064E+11 0.3078E+11 0.2277E+11 0.1677E+11
0.1215E+11 0.8655E+10 0.6124E+10 0.4247E+10 0.2925E+10
0.1960E+10 0.1273E+10 0.8155E+09 0.4922E+09 0.2925E+09
0.1707E+09 0.9796E+08 0.5558E+08 0.3120E+08 0.1748E+08
0.1014E+08 0.6111E+07 0.3726E+07 0.2433E+07 0.1609E+07
0.1070E+07 0.7147E+06 0.4819E+06 0.3331E+06 0.2326E+06
0.1635E+06 0.1159E+06 0.8362E+05 0.6619E+05 0.5362E+05
0.4420E+05 0.3697E+05 0.3130E+05 0.2678E+05 0.2312E+05
0.2012E+05 0.1763E+05 0.1555E+05 0.1379E+05 0.1228E+05
0.1100E+05 0.9884E+04 0.8916E+04 0.5574E+04 0.3689E+04
0.2542E+04 0.1804E+04 0.1310E+04 0.9686E+03 0.7269E+03
0.5524E+03 0.4243E+03 0.3291E+03 0.2574E+03 0.2028E+03
0.1609E+03 0.1285E+03 0.1033E+03
END
CH4 DENSITIES
0.3145E+14 0.2795E+14 0.2492E+14 0.2226E+14 0.1987E+14
0.1768E+14 0.1569E+14 0.1384E+14 0.1214E+14 0.1057E+14
0.9147E+13 0.7859E+13 0.6716E+13 0.5720E+13 0.4863E+13
0.4130E+13 0.3512E+13 0.2987E+13 0.2540E+13 0.2160E+13
0.1836E+13 0.1560E+13 0.1324E+13 0.1124E+13 0.9529E+12
0.6845E+12 0.4908E+12 0.3515E+12 0.2246E+12 0.1405E+12
0.8649E+11 0.5223E+11 0.3014E+11 0.2118E+11 0.1494E+11
0.1077E+11 0.7941E+10 0.5881E+10 0.4398E+10 0.3290E+10
0.2464E+10 0.1846E+10 0.1378E+10 0.1029E+10 0.7651E+09
0.5662E+09 0.4171E+09 0.3048E+09 0.2219E+09 0.1602E+09
0.1150E+09 0.8175E+08 0.5727E+08 0.3968E+08 0.2703E+08
0.1814E+08 0.1201E+08 0.7851E+07 0.5113E+07 0.3319E+07
0.2163E+07 0.1421E+07 0.9427E+06 0.6355E+06 0.4335E+06
0.2994E+06 0.2093E+06 0.1475E+06 0.1051E+06 0.7550E+05
0.5493E+05 0.4055E+05 0.3042E+05 0.2408E+05 0.1950E+05
0.1608E+05 0.1345E+05 0.1138E+05 0.9740E+04 0.8409E+04
0.7318E+04 0.6413E+04 0.5655E+04 0.5014E+04 0.4469E+04
0.4000E+04 0.3595E+04 0.3243E+04 0.2028E+04 0.1342E+04
0.9246E+03 0.6562E+03 0.4765E+03 0.3523E+03 0.2644E+03
0.2009E+03 0.1544E+03 0.1197E+03 0.9361E+02 0.7377E+02
0.5854E+02 0.4675E+02 0.3758E+02
END
HNO3 DENSITIES
0.9718E+10 0.9994E+10 0.1032E+11 0.1068E+11 0.1105E+11
0.1140E+11 0.1172E+11 0.1198E+11 0.1218E+11 0.1229E+11

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0.1232E+11 0.1229E+11 0.1217E+11 0.1202E+11 0.1184E+11
0.1167E+11 0.1152E+11 0.1137E+11 0.1121E+11 0.1425E+11
0.1371E+11 0.1271E+11 0.1146E+11 0.1016E+11 0.8738E+10
0.5648E+10 0.3339E+10 0.1972E+10 0.1032E+10 0.5408E+09
0.2664E+09 0.1237E+09 0.5785E+08 0.2725E+08 0.1296E+08
0.6219E+07 0.3012E+07 0.1468E+07 0.7188E+06 0.3527E+06
0.1731E+06 0.8488E+05 0.4154E+05 0.2027E+05 0.9853E+04
0.4767E+04 0.2294E+04 0.1096E+04 0.5205E+03 0.2454E+03
0.1150E+03 0.5331E+02 0.2439E+02 0.1099E+02 0.4878E+01
0.2132E+01 0.9196E+00 0.3921E+00 0.1658E+00 0.6994E-01
0.2962E-01 0.1264E-01 0.5460E-02 0.2390E-02 0.1060E-02
0.4754E-03 0.2156E-03 0.9870E-04 0.4559E-04 0.2127E-04
0.1005E-04 0.4813E-05 0.2345E-05 0.1856E-05 0.1504E-05
0.1240E-05 0.1037E-05 0.8777E-06 0.7509E-06 0.6483E-06
0.5642E-06 0.4944E-06 0.4360E-06 0.3866E-06 0.3445E-06
0.3084E-06 0.2772E-06 0.2500E-06 0.1563E-06 0.1035E-06
0.7128E-07 0.5059E-07 0.3674E-07 0.2716E-07 0.2039E-07
0.1549E-07 0.1190E-07 0.9228E-08 0.7217E-08 0.5688E-08
0.4513E-08 0.3605E-08 0.2897E-08
END
N2O DENSITIES
0.7863E+13 0.7048E+13 0.6342E+13 0.5715E+13 0.5147E+13
0.4625E+13 0.4139E+13 0.3686E+13 0.3263E+13 0.2869E+13
0.2506E+13 0.2174E+13 0.1876E+13 0.1616E+13 0.1382E+13
0.1170E+13 0.9778E+12 0.8067E+12 0.6664E+12 0.5502E+12
0.4507E+12 0.3702E+12 0.3041E+12 0.2459E+12 0.2021E+12
0.1206E+12 0.7217E+11 0.4318E+11 0.2054E+11 0.9783E+10
0.4549E+10 0.2070E+10 0.9478E+09 0.5188E+09 0.2865E+09
0.1736E+09 0.1154E+09 0.7721E+08 0.5336E+08 0.3697E+08
0.2538E+08 0.1725E+08 0.1170E+08 0.7942E+07 0.5372E+07
0.3624E+07 0.2436E+07 0.1627E+07 0.1073E+07 0.7036E+06
0.4586E+06 0.2960E+06 0.1885E+06 0.1186E+06 0.7345E+05
0.4474E+05 0.2684E+05 0.1592E+05 0.9373E+04 0.5508E+04
0.3250E+04 0.1934E+04 0.1164E+04 0.7097E+03 0.4382E+03
0.2736E+03 0.1725E+03 0.1099E+03 0.7072E+02 0.4600E+02
0.3048E+02 0.2062E+02 0.1419E+02 0.1123E+02 0.9099E+01
0.7501E+01 0.6274E+01 0.5311E+01 0.4544E+01 0.3923E+01
0.3414E+01 0.2992E+01 0.2638E+01 0.2339E+01 0.2085E+01
0.1866E+01 0.1677E+01 0.1513E+01 0.9460E+00 0.6260E+00
0.4313E+00 0.3061E+00 0.2223E+00 0.1644E+00 0.1234E+00
0.9374E-01 0.7201E-01 0.5584E-01 0.4367E-01 0.3442E-01
0.2731E-01 0.2181E-01 0.1753E-01
END
NO2 DENSITIES
0.1767E+10 0.1838E+10 0.1919E+10 0.2010E+10 0.2099E+10
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0.2188E+10 0.2273E+10 0.2349E+10 0.2414E+10 0.2464E+10
0.2500E+10 0.2516E+10 0.2520E+10 0.2515E+10 0.2504E+10
0.2496E+10 0.2489E+10 0.2482E+10 0.2475E+10 0.2468E+10
0.2470E+10 0.2419E+10 0.2421E+10 0.2474E+10 0.2598E+10
0.2692E+10 0.2656E+10 0.2618E+10 0.2080E+10 0.1654E+10
0.1235E+10 0.8673E+09 0.6131E+09 0.3932E+09 0.2544E+09
0.1593E+09 0.9645E+08 0.5877E+08 0.2928E+08 0.1462E+08
0.7307E+07 0.3648E+07 0.1818E+07 0.9037E+06 0.4474E+06
0.2205E+06 0.1080E+06 0.5258E+05 0.2541E+05 0.1220E+05
0.5816E+04 0.2745E+04 0.1278E+04 0.5869E+03 0.2653E+03
0.1181E+03 0.5187E+02 0.2252E+02 0.9702E+01 0.4172E+01
0.1801E+01 0.7844E+00 0.3455E+00 0.1547E+00 0.7018E-01
0.3237E-01 0.1516E-01 0.7170E-02 0.3512E-02 0.1738E-02
0.7663E-03 0.3018E-03 0.1209E-03 0.9568E-04 0.7750E-04
0.6389E-04 0.5344E-04 0.4524E-04 0.3870E-04 0.3341E-04
0.2908E-04 0.2548E-04 0.2247E-04 0.1993E-04 0.1776E-04
0.1589E-04 0.1429E-04 0.1289E-04 0.8058E-05 0.5333E-05
0.3674E-05 0.2608E-05 0.1893E-05 0.1400E-05 0.1051E-05
0.7985E-06 0.6134E-06 0.4757E-06 0.3720E-06 0.2932E-06
0.2326E-06 0.1858E-06 0.1493E-06
END
SO2 DENSITIES
0.7847E+10 0.6424E+10 0.4979E+10 0.3612E+10 0.2500E+10
0.1815E+10 0.1337E+10 0.1018E+10 0.7825E+09 0.6261E+09
0.5068E+09 0.4187E+09 0.3494E+09 0.3000E+09 0.2599E+09
0.2274E+09 0.1953E+09 0.1567E+09 0.1199E+09 0.8555E+08
0.5905E+08 0.4244E+08 0.3110E+08 0.2422E+08 0.1906E+08
0.1225E+08 0.8097E+07 0.5312E+07 0.3590E+07 0.2516E+07
0.1851E+07 0.1437E+07 0.1174E+07 0.1028E+07 0.9348E+06
0.8788E+06 0.8410E+06 0.7975E+06 0.6879E+06 0.5947E+06
0.5003E+06 0.4090E+06 0.3337E+06 0.2585E+06 0.1994E+06
0.1483E+06 0.1062E+06 0.7558E+05 0.4822E+05 0.3055E+05
0.1800E+05 0.9824E+04 0.5291E+04 0.2678E+04 0.1335E+04
0.6504E+03 0.3102E+03 0.1461E+03 0.6802E+02 0.3156E+02
0.1467E+02 0.6866E+01 0.3246E+01 0.1553E+01 0.7523E+00
0.3686E+00 0.1825E+00 0.9117E-01 0.4588E-01 0.2333E-01
0.1201E-01 0.6280E-02 0.3340E-02 0.2616E-02 0.2097E-02
0.1712E-02 0.1419E-02 0.1190E-02 0.1009E-02 0.8643E-03
0.7461E-03 0.6487E-03 0.5676E-03 0.4995E-03 0.4418E-03
0.3925E-03 0.3502E-03 0.3136E-03 0.1891E-03 0.1205E-03
0.7986E-04 0.5438E-04 0.3778E-04 0.2665E-04 0.1901E-04
0.1368E-04 0.9916E-05 0.7227E-05 0.5291E-05 0.3887E-05
0.2865E-05 0.2117E-05 0.1568E-05
END
NH3 DENSITIES

0.1308E+11 0.1172E+11 0.9768E+10 0.7225E+10 0.4931E+10
0.3138E+10 0.2010E+10 0.1211E+10 0.7033E+09 0.3598E+09
0.1692E+09 0.7881E+08 0.3931E+08 0.1675E+08 0.5115E+07
0.1768E+07 0.7167E+06 0.3210E+06 0.1680E+06 0.8555E+05
0.4461E+05 0.3052E+05 0.2346E+05 0.1860E+05 0.1445E+05
0.8129E+04 0.4687E+04 0.2517E+04 0.1193E+04 0.5144E+03
0.2180E+03 0.8541E+02 0.2539E+02 0.7202E+01 0.2245E+01
0.8011E+00 0.3329E+00 0.1597E+00 0.1062E+00 0.7083E-01
0.4843E-01 0.3393E-01 0.2372E-01 0.1702E-01 0.1216E-01
0.8730E-02 0.6286E-02 0.4496E-02 0.3233E-02 0.2308E-02
0.1644E-02 0.1163E-02 0.8115E-03 0.5600E-03 0.3804E-03
0.2555E-03 0.1698E-03 0.1115E-03 0.7276E-04 0.4731E-04
0.3084E-04 0.2024E-04 0.1342E-04 0.9066E-05 0.6199E-05
0.4282E-05 0.2985E-05 0.2100E-05 0.1493E-05 0.1072E-05
0.7798E-06 0.5763E-06 0.4335E-06 0.3394E-06 0.2722E-06
0.2222E-06 0.1841E-06 0.1545E-06 0.1310E-06 0.1122E-06
0.9682E-07 0.8418E-07 0.7366E-07 0.6482E-07 0.5733E-07
0.5094E-07 0.4545E-07 0.4070E-07 0.2453E-07 0.1564E-07
0.1036E-07 0.7058E-08 0.4903E-08 0.3458E-08 0.2467E-08
0.1776E-08 0.1287E-08 0.9379E-09 0.6866E-09 0.5045E-09
0.3718E-09 0.2748E-09 0.2035E-09
END